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RAYLEIGH-BLOCH WAVE EXPANSIONS FOR DIFFRACTION GRATINGS I.(U)
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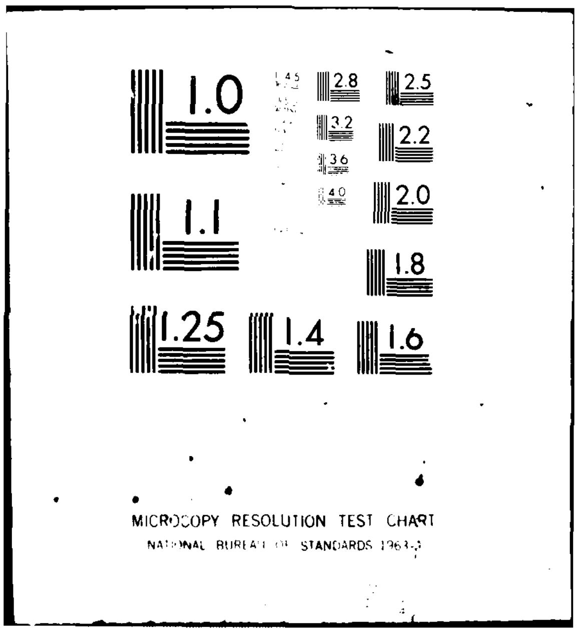
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Rayleigh-Bloch Wave Expansions

for Diffraction Gratings I.

10 Calvin H. Wilcox

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Abstract.

Plane diffraction gratings with period 2π lying in a strip $0 < y < h$ in the x,y-plane are studied. A Rayleigh-Bloch (R-B) wave for a grating is the response $\psi_+(x,y,p,q)$ to a plane wave $(2\pi)^{-1}\exp(i(px-qy))$ incident from $y > h$ ($p \in R$, $q > 0$). Thus $(\Delta + (p^2 + q^2))\,\psi_+ = 0$ in the domain G above the grating, ψ_+ satisfies the Dirichlet or Neumann boundary condition on ∂G and for $y > h$

Psi sub +

delta

1/2 p1

$$\psi_+(x,y,p,q) = (2\pi)^{-1} \exp\{i(px - qy)\}$$

$$+ \sum_{(p+\ell)^2<p^2+q^2} c_\ell^+(p,q) \exp\{i\, p_\ell\, x + q_\ell\, y\}$$

$$+ \sum_{(p+\ell)^2\geq p^2+q^2} c_\ell^+(p,q) \exp\{i\, p_\ell x - ((p+\ell)^2 - p^2 - q^2)^{1/2}\ y\}$$

where $(p_\ell, q_\ell) = (p + \ell, (p^2 + q^2 - (p + \ell)^2)^{1/2})$ and the summations are over all integers ℓ satisfying the indicated inequalities. The paper presents a construction of R-B waves and a proof that

eta

$\{\psi_+(x,y,p,q) \mid p \in R,\ q > 0\}$ is a complete orthogonal family in $L_2(G)$ in the sense of the Plancherel theory.

psi sub +

Introduction.

The phenomena associated with the scattering of acoustic and electromagnetic waves by periodic surfaces play a role in many areas of applied physics and engineering. Optical gratings date from the nineteenth century and are still used by spectroscopists. More recently, gratings have been used as coupling devices in integrated optics [5]. Trains of surface waves on the oceans are natural diffraction gratings which influence the scattering of electromagnetic waves [31] and underwater sound [13]. Similarly, the surface of a crystal acts as a diffraction grating for the scattering of atomic beams [14]. The literature on diffraction gratings and their applications is very large. References to work done before 1967 may be found in the monograph by Stroke in the <u>Handbuch der Physik</u> [29]. More recent references are given in the papers of Fortuin [13], Millar [20], Jordan and Lang [16] and De Santo [9], among others.

The first theoretical studies of scattering by diffraction gratings are due to Rayleigh. His "Theory of Sound" Volume 2, 2nd Edition, published in 1896 [22], contains an analysis of the scattering of a monochromatic plane wave normally incident on a grating with a sinusoidal profile. In a subsequent paper [23] he extended the analysis to oblique incidence. Rayleigh assumed in his work that in the half-space above the grating the reflected wave is a superposition of the specularly reflected plane wave, a finite number of secondary plane waves propagating in the directions of the higher order grating spectra of optics, and an infinite sequence of evanescent waves whose amplitudes decrease exponentially with distance from the grating. The validity of Rayleigh's assumption for general grating profiles was realized in the early 1930's [11], following Bloch's work [4] on the analogous problem of de Broglie waves in crystals. Waves of this type will be called Rayleigh-Bloch waves (R-B waves for brevity) in this report.

The goal of Rayleigh's work and the literature based on it was to calculate the relative amplitudes and phases of the components of the R-B waves and several methods for doing this have been developed. L. A. Weinstein [32] and J. A. De Santo [6, 7] have given exact solutions to the problem of the scattering of monochromatic plane waves by a comb grating; i.e., an array of periodically spaced infinitesimally thin parallel plates of finite depth mounted perpendicularly on a plane. For gratings with sinusoidal profiles, infinite systems of linear equaltions for the complex reflection coefficients have been given by J. L. Uretsky [30] and J. A. De Santo [8]. Numerical solutions of these equations have been given by A. K. Jordan and R. H. Lang [16] whose paper contains references to numerical work by other authors.

The work referenced above provides a satisfactory understanding of the scattering of the steady beams used in classical spectroscopy. However, modern applications of gratings in areas such as integrated optics and underwater sound require an understanding of how transient electromagnetic and acoustic fields, such as pulsed laser beams and sonar signals, are scattered by diffraction gratings. The existing theory of R-B waves is inadequate for the analysis of these problems.

The purpose of this report is to present an eigenfunction expansion for diffraction gratings in which the eigenfunctions are R-B waves. The theory can be used to analyze the scattering of transient fields by diffraction gratings. The analysis, which parallels the author's work on the scattering of transient sound waves by bounded obstacles [34, 35, 37] will be given in a separate report.

The theory of R-B wave expansions given below is a generalization of T. Ikebe's theory of distorted plane wave expansions [15], first developed for quantum mechanical potential scattering and subsequently extended to a variety of scattering problems [2, 19, 25, 26, 27, 35]. The theory is based on the study of a linear operator A, called here the grating propagator, which is a selfadjoint realization of the negative Laplacian acting in the Hilbert space of square integrable acoustic fields. The principal result of this report is a representation of the spectral family of A by means of R-B waves. The R-B wave expansions follow as a corollary.

A key step in developing R-B wave expansions is the introduction of the reduced grating propagator A_p which depends on the wave momentum p. The Hilbert space theory of such operators was initiated in a recent article by H. D. Alber [3]. Here Alber's powerful method of analytic continuation of the resolvent of A_p is used to construct the R-B wave eigenfunctions.

The derivation of the R-B wave expansions given below is restricted, for brevity, to the case of two-dimensional wave propagation. Specifically, the waves are assumed to be solutions of the wave equation in a two-dimensional grating domain and to satisfy the Dirichlet or Neumann boundary condition on the grating profile. These problems provide models for the scattering of sound waves by acoustically soft or rigid gratings and of TE or TM electromagnetic waves by perfectly conducting gratings. It will be seen that the methods employed are also applicable to three-dimensional (and n-dimensional) grating problems.

Even with the restriction to the two-dimensional case, the analytical work needed to derive and fully establish eigenfunction expansions for diffraction gratings is necessarily intricate and lengthy. This is clear from examination of the simpler case of scattering by bounded obstacles presented in the author's monograph [34]. Therefore, to make the work accessible to potential users, this report presents only the concepts and results of the theory, together with the principal ideas needed to derive them. Complete analytical details and proofs are provided in a companion report.

The remainder of this report is organized as follows. §1 contains the definitions of the class of grating domains and corresponding grating propagators. §2 contains the definition of the R-B waves and their classification into surface waves and diffracted plane waves. The concept of the reduced grating propagator A_p is introduced in §3 and the R-B surface and diffracted plane waves are shown to be eigenfunctions and generalized eigenfunctions, respectively, of A_p. The section includes the spectral analysis of the reduced propagator $A_{0,p}$ corresponding to the degenerate grating whose profile is a straight line. In subsequent sections the R-B wave expansions for general gratings are developed as perturbations of this special case.

In §4 the analytic continuation of the resolvent of A_p to a suitable Riemann surface is constructed by the method of Alber. The method leads to a particularly strong form of the limiting absorption principle. In §5 the results of §4 are used to construct the R-B eigenfunctions for A_p and to derive corresponding spectral representations and eigenfunction expansions for A_p. In §6 these results are used to construct the corresponding R-B wave spectral representations and eigenfunction expansions for the grating propagator A. §7 contains concluding remarks concerning extensions of the theory and unsolved problems.

(1.1), (1.2) can be written

(1.6) $$R_h^2 \subset G \subset R_0^2 \text{ for some } h > 0$$

and the translation invariance (1.3) takes the form

(1.7) $$G + (a,0) = G$$

where $a > 0$ is the primitive period of G.

The eigenfunction expansion theory for R-B waves that satisfy the Dirichlet boundary condition is developed below for arbitrary grating domains. For R-B waves that satisfy the Neumann boundary condition the following additional conditions are imposed on ∂G, the frontier of G.

(1.8) G has the local compactness property, and

(1.9) there exists an $x_0 \in R$ such that the set $\partial G \cap \{(x_0,y) \mid y \geq 0\}$ is finite and each (x_0,y) in the set has a neighborhood in R^2 in which ∂G is a regular curve of class C^3.

Condition (1.8) was introduced in [34] where it was denoted by $G \in LC$. It is a mild regularity property of ∂G. A simple sufficient condition for $G \in LC$ is the "finite tiling condition" of [34, p. 63]. Grating domains that satisfy (1.8) and (1.9) will be said to have property S, written $G \in S$. The class includes all the piece-wise smooth gratings that arise in applications. Examples include the domains $G = \{X \mid y > h(x)\}$ where $h(x)$ is bounded, piece-wise smooth and has period a. A special case is De Santo's comb grating for which

§1. Grating Domains and Grating Propagators.

The plane diffraction gratings that are studied in this report are the boundaries of the class of planar domains G defined by the following properties.

(1.1) G is contained in a half-plane.

(1.2) G contains a smaller half-plane.

(1.3) G is invariant under translation through a distance $a > 0$.

Domains with these properties will be called grating domains. The half-plane of (1.2) is necessarily parallel to that of (1.1) and the translation of (1.3) is necessarily parallel to the edges of these half-planes. The smallest $a > 0$ for which (1.3) holds is called the primitive grating period. It exists for all gratings except the degenerate grating for which G is a half-plane.

It will be convenient to introduce Cartesian coordinates

$$X = (x,y) \in R^2 \tag{1.4}$$

in the plane of G such that the x-axis is parallel to the edges of the half-planes of (1.1), (1.2) and to identify G with the corresponding domain (open connected set) $G \subset R^2$. With this convention if

$$R_c^2 = \{X \in R^2 \mid y > c\} \tag{1.5}$$

then, for a suitable orientation of the coordinate axes, conditions

(1.1), (1.2) can be written

(1.6) $$R^2_h \subset G \subset R^2_0 \text{ for some } h > 0$$

and the translation invariance (1.3) takes the form

(1.7) $$G + (a,0) = G$$

where $a > 0$ is the primitive period of G.

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$$h(x) = \begin{cases} h > 0 \text{ for } x = 0 \\ 0 \text{ for } -a/2 \le x < 0 \text{ and } 0 < x \le a/2 \end{cases} \tag{1.10}$$

The Hilbert space theory of solutions of the wave equation in arbitrary domains $G \subset R^n$, developed by the author in [33, 34], provides the foundation for the analysis of scattering by diffraction gratings given below. The basic Hilbert space of the theory is the Lebesgue space $L_2(G)$ with scalar product

$$(u,v) = \int_G \overline{u(X)}\, v(X)\, dX \tag{1.11}$$

In addition, the definition of the grating propagators makes use of the Sobolev spaces

$$L_2^m(G) = L_2(G) \cap \{u \mid D_1^{\alpha_1} D_2^{\alpha_2} u \in L_2(G) \text{ for } \alpha_1 + \alpha_2 \le m\} , \tag{1.12}$$

where $D_1 = \partial/\partial x$, $D_2 = \partial/\partial y$ and m is a positive integer, and the space

$$L_2^1(\Delta,G) = L_2^1(G) \cap \{u \mid \Delta u \in L_2(G)\} \tag{1.13}$$

where $\Delta = D_1^2 + D_2^2$ is the Laplacian in R^2. In these definitions the differential operators are to be interpreted in the distribution-theoretic sense (cf. [33, 34]).

The grating propagators for a grating domain G are selfadjoint realizations in $L_2(G)$ of $-\Delta$, acting on sets of functions that satisfy the Neumann or Dirichlet boundary conditions. These operators will be denoted by $A^N(G)$ and $A^D(G)$, respectively. Their domains are subsets of $L_2^1(\Delta,G)$ that satisfy the boundary conditions in a form appropriate to arbitrary domains G. In particular, functions $u \in D(A^N(G))$ are required to satisfy the generalized Neumann condition

$$\int_G \{(\Delta u)\overline{v} + \nabla u \cdot \nabla\overline{v}\}\, dX = 0 \tag{1.14}$$

for all $v \in L_2^1(G)$. In fact, if one defines

$$L_2^N(\Delta,G) = L_2^1(\Delta,G) \cap \{u \mid (1.14) \text{ holds for all } v \in L_2^1(G)\}\ , \tag{1.15}$$

$D(A^N(G)) = L_2^N(\Delta,G)$ and $A^N(G)u = -\Delta u$ then $A^N(G)$ is a selfadjoint non-negative operator in $L_2(G)$. This characterization was proved in [34]. It may also be derived from T. Kato's theory of sesquilinear forms in Hilbert space [17, Ch. 6]. It is known that if ∂G is a smooth curve then $D(A^N(G)) \subset L_2^2(G)$ and ∇u has a trace in $L_2(\partial G)$ which satisfies the Neumann boundary condition [34].

To define the grating propagator $A^D(G)$ associated with the Dirichlet boundary condition let

$$L_2^D(G) = \text{closure of } C_0^\infty(G) \text{ in } L_2^1(G) \tag{1.16}$$

and define

$$L_2^D(\Delta,G) = L_2^D(G) \cap L_2^1(\Delta,G)\ , \tag{1.17}$$

$D(A^D(G)) = L_2^D(\Delta,G)$ and $A^D(G)u = -\Delta u$. Then Kato's theory of sesquilinear forms may be used to show that $A^D(G)$ is also a selfadjoint non-negative operator in $L_2(G)$. Moreover, it is known that if ∂G is a smooth curve then every $u \in L_2^1(G)$ has a trace $u|\partial G \in L_2(\partial G)$ and every $u \in L_2^D(G)$ satisfies $u|\partial G = 0$ [18].

The grating propagators $A^N(G)$ and $A^D(G)$ will be shown to have pure continuous spectra. It follows that the R-B wave eigenfunctions must be generalized eigenfunctions which are not in $L_2(G)$. To define them it will be convenient to define extensions of $A^N(G)$ and $A^D(G)$ which act in the space

$$(1.18) \qquad L_2^{\ell oc}(G) = \mathcal{D}'(G) \cap \{u \mid u \in L_2(K \cap G) \text{ for all compact } K \subset R^2\}$$

where $\mathcal{D}'(G)$ is the set of all distributions on G. The following subsets of $L_2^{\ell oc}(G)$ are also needed:

$$(1.19) \qquad L_2^{m,\ell oc}(G) = L_2^{\ell oc}(G) \cap \{u \mid D_1^{\alpha_1} D_2^{\alpha_2} u \in L_2^{\ell oc}(G) \text{ for } \alpha_1 + \alpha_2 \le m\} ,$$

$$(1.20) \qquad L_2^{1,\ell oc}(\Delta,G) = L_2^{1,\ell oc}(G) \cap \{u \mid \Delta u \in L_2^{\ell oc}(G)\} .$$

These linear spaces are all Fréchet spaces (locally convex topological vector spaces which are metrizable and complete [10]) under suitable definitions of the topologies. Thus $L_2^{\ell oc}(G)$ is a Fréchet space with family of semi-norms

$$(1.21) \qquad \rho_K(u) = \left(\iint_{K \cap G} |u(X)|^2 \, dX\right)^{1/2}$$

indexed by the compact sets $K \subset R^2$. Similarly, $L_2^{m,\ell oc}(G)$ is a Fréchet space with family of semi-norms

$$(1.22) \qquad \rho_K(u) = \left(\iint_{K \cap G} \sum_{\alpha_1+\alpha_2 \le m} |D_1^{\alpha_1} D_2^{\alpha_2} u(X)|^2 \, dX\right)^{1/2}$$

and $L_2^{1,\ell oc}(\Delta,G)$ is a Fréchet space with family of semi-norms

$$(1.23) \qquad \rho_K(u) = \left(\iint_{K \cap G} \{|u(X)|^2 + |\nabla u(X)|^2 + |\Delta u(X)|^2\} \, dX\right)^{1/2}$$

The following additional notation is used below:

$$(1.24) \qquad L_2^{com}(G) = L_2(G) \cap \mathcal{E}'(R^2)$$

$$L_2^{1,com}(G) = L_2^1(G) \cap L_2^{com}(G) \tag{1.25}$$

where $\mathcal{E}'(R^2)$ denotes the set of all distributions on R^2 with compact supports.

The local grating propagator $A^{N,\ell oc}(G)$ for G and the Neumann boundary condition is the extension of $A^N(G)$ in $L_2^{\ell oc}(G)$ defined by

$$\begin{aligned} D(A^{N,\ell oc}(G)) &= L_2^{N,\ell oc}(\Delta,G) \\ &\equiv L_2^{1,\ell oc}(\Delta,G) \cap \{u \mid (1.14) \text{ holds for all } v \in L_2^{1,com}(G)\} \end{aligned} \tag{1.26}$$

and

$$A^{N,\ell oc}(G)u = -\Delta u \text{ for all } u \in D(A^{N,\ell oc}(G)) . \tag{1.27}$$

Similarly, the local grating propagator $A^{D,\ell oc}(G)$ for G and the Dirichlet boundary condition is the extension of $A^D(G)$ in $L_2^{\ell oc}(G)$ defined by

$$D(A^{D,\ell oc}(G)) = L_2^{D,\ell oc}(\Delta,G) \equiv L_2^{D,\ell oc}(G) \cap L_2^{1,\ell oc}(\Delta,G) \tag{1.28}$$

where

$$L_2^{D,\ell oc}(G) = \text{Closure of } C_0^\infty(G) \text{ in } L_2^{1,\ell oc}(G) \tag{1.29}$$

and

$$A^{D,\ell oc}(G)u = -\Delta u \text{ for all } u \in D(A^{D,\ell oc}(G)). \tag{1.30}$$

The spectral analysis and eigenfunction expansions for $A^N(G)$ and $A^D(G)$ are nearly identical. To emphasize this, and to simplify the notation, the symbol A will be used to denote either $A^N(G)$ or $A^D(G)$ in stating results that are valid for both. Similarly, the symbol $A^{\ell oc}$ will denote $A^{N,\ell oc}(G)$ or $A^{D,\ell oc}(G)$ except where a distinction is necessary.

The spectral theory of $A^N(G)$ and $A^D(G)$ will be developed by perturbation theory, beginning with the degenerate grating R_0^2. The grating propagators for this case will be denoted by

$$(1.31) \qquad A_0^N = A^N(R_0^2), \qquad A_0^D = A^D(R_0^2)$$

and

$$(1.32) \qquad A_0^{N,\ell oc} = A^{N,\ell oc}(R_0^2), \qquad A_0^{D,\ell oc} = A^{D,\ell oc}(R_0^2)$$

and the condensed notation A_0 for A_0^N or A_0^D and $A_0^{\ell oc}$ for $A_0^{N,\ell oc}$ or $A_0^{D,\ell oc}$ will be used.

The spectral analysis of A_0 can be carried out by separation of variables and is essentially elementary. Thus D_1^2 is essentially selfadjoint in $L_2(R)$ with complete family of generalized eigenfunctions $\{(2\pi)^{-1/2} \exp(ipx) \mid p \in R\}$. Similarly, D_2^2 and the Neumann boundary condition define a selfadjoint operator in $L_2(0,\infty)$ with complete family $\{(2/\pi)^{1/2} \cos q\, y \mid q > 0\}$, while D_2^2 and the Dirichlet boundary condition define a second selfadjoint operator in $L_2(0,\infty)$ with complete family $\{(2/\pi)^{1/2} \sin q\, y \mid q > 0\}$. It follows that the products

$$(1.33) \qquad \psi_0^N(X,p,q) = \frac{1}{\pi} e^{ip\cdot x} \cos q\, y\ , \quad (p,q) \in R_0^2$$

$$(1.34) \qquad \psi_0^D(X,p,q) = \frac{1}{\pi} e^{ip\cdot x} \sin q\, y\ , \quad (p,q) \in R_0^2$$

are in $D(A_0^{N,\ell oc})$ and $D(A_0^{D,\ell oc})$, respectively, and define complete families of generalized eigenfunctions for A_0^N and A_0^D. More precisely, if ψ_0 is used to denote either ψ_0^N or ψ_0^D then the classical Plancherel theory can be used to derive an eigenfunction expansion and spectral decomposition for

$$A_0 = \int_0^\infty \mu \, d\Pi_0(\mu) \tag{1.35}$$

which may be formulated as follows. First, for all $f \in L_2(R_0^2)$ the limit

$$\hat{f}_0(p,q) = L_2(R_0^2)\text{-}\lim_{M\to\infty} \int_0^M \int_{-M}^M \overline{\psi_0(X,p,q)} \, f(X) \, dX \tag{1.36}$$

exists and

$$f(X) = L_2(R_0^2)\text{-}\lim_{M\to\infty} \int_0^M \int_{-M}^M \psi_0(X,p,q) \, \hat{f}_0(p,q,) \, dpdq \tag{1.37}$$

and

$$\|f\|_{L_2(R_0^2)} = \|\hat{f}_0\|_{L_2(R_0^2)} \ . \tag{1.38}$$

Moreover, the spectral family of A_0 is given by

$$\Pi_0(\mu) \; f(X) = \int_{\{(p,q)\,|\,p^2+q^2\le\mu, q>0\}} \psi_0(X,p,q) \, \hat{f}_0(p,q) \, dpdq \ . \tag{1.39}$$

Finally, if the linear operator $\Phi_0 : L_2(R_0^2) \to L_2(R_0^2)$ is defined by $\Phi_0 f = \hat{f}_0$ then Φ_0 is unitary.

The principal result of this report is a generalization of this eigenfunction expansion and spectral analysis that is valid for the operator $A^D(G)$ in arbitrary grating domains G and for the operator $A^N(G)$ in grating domains $G \in S$. In these generalizations the R-B waves play the role of the eigenfunctions ψ_0.

§2. Rayleigh-Bloch Waves.

It will be assumed in the remainder of the report that the unit of length has been chosen to make the grating period $a = 2\pi$. This normalization, which simplifies many of the equations, does not limit the generality of the theory because the general case can be recovered by a simple change of units.

The definition of the R-B waves can be motivated by considering the reflection by a grating of a plane wave

$$(2.1) \qquad \psi^{inc}(X,p,q) = (2\pi)^{-1} \exp \{i(px - qy)\}, \ (p,q) \in R_0^2 \ .$$

Note that the effect of translating ψ^{inc} by the grating period 2π is to multiply it by a factor of modulus 1:

$$(2.2) \qquad \psi^{inc}(x + 2\pi,y,p,q) = \exp \{2\pi ip\} \ \psi^{inc}(x,y,p,q) \ .$$

Since G is invariant under this translation the reflected wave, if it is uniquely determined by ψ^{inc}, must also have property (2.2). This suggests the

<u>Definition</u>. A function $\psi \in L_2^{1,\ell oc}(\Delta,G)$ is said to be an R-B wave for G if and only if there exist numbers $p \in R$ and $\omega \geq 0$ such that

$$(2.3) \qquad \psi(x + 2\pi,y) = \exp \{2\pi ip\} \ \psi(x,y) \text{ in } G \ ,$$

$$(2.4) \qquad \Delta\psi + \omega^2\psi = 0 \text{ in } G, \text{ and}$$

$$(2.5) \qquad \psi(X) \text{ is bounded in } G.$$

If, in addition,

$$\psi \in D(A^{\ell oc}) \tag{2.6}$$

then ψ is said to be an R-B wave for A.

The parameters ω and p will be called the frequency and x-momentum of the R-B wave, respectively. Note that p is only determined modulo 1 by (2.6). The x-momentum that satisfies

$$-1/2 < p \leq 1/2 \tag{2.7}$$

will be called the reduced x-momentum of ψ. Property (2.3) is sometimes called quasi-periodicity or p-periodicity. It is equivalent to the property that

$$\psi(x,y) = \exp\{ipx\}\, \phi(x,y) \text{ for all } (x,y) \in G \tag{2.8}$$

where

$$\phi(x + 2\pi, y) = \phi(x,y) \text{ for all } (x,y) \in G \,. \tag{2.9}$$

Solutions of the Helmholtz equation (2.4) are known to be analytic functions. In particular, each R-B wave for A satisfies $\psi \in C^{\infty}(G)$. Hence, the function ϕ in (2.8) is in $C^{\infty}(R^2_h)$ and has period 2π in x. In follows from classical convergence theory for Fourier series that ψ has an expansion

$$\psi(x,y) = \sum_{\ell \in Z} \psi_{\ell}(y) \exp\{i(p + \ell)x\},\ (x,y) \in R^2_h \,, \tag{2.10}$$

where Z denotes the set of all integers. The series converges absolutely and uniformly on compact subsets of R^2_h. Moreover, the partial derivatives of ψ have expansions of the same form which may be calculated from (2.10) by term-by-term differentiation and which have the same convergence properties. It follows that the coefficients $\psi_\ell(y)$ in (2.10) must satisfy

$$\psi_\ell''(y) + (\omega^2 - (p+\ell)^2)\,\psi_\ell(y) = 0 \text{ for } y > h\ . \tag{2.11}$$

Hence the terms in the expansion (2.10) have the following forms, depending on the relative magnitudes of ω and $|p+\ell|$.

$\underline{\omega > |p+\ell|}$. In this case there exist constants c_ℓ^+ and c_ℓ^- such that

$$\psi_\ell(y)\exp\{i(p+\ell)x\} = c_\ell^+\exp\{i(p_\ell x + q_\ell y)\} + c_\ell^-\exp\{i(p_\ell x - q_\ell y)\} \tag{2.12}$$

where

$$p_\ell = p+\ell,\ q_\ell = (\omega^2 - (p+\ell)^2)^{1/2} > 0\ . \tag{2.13}$$

the two terms in (2.12) describe plane waves propagating in the directions $(p_\ell, \pm q_\ell)$. Since $p_\ell^2 + q_\ell^2 = \omega^2$ these vectors lie on the circle of radius ω with center at the origin and their x-components differ by integers. Clearly there are only finitely many such terms.

$\underline{\omega < |p+\ell|}$. In this case $\psi_\ell(y)$ is a linear combination of real exponentials in y and the boundedness condition (2.5) implies that

$$\psi_\ell(y)\exp\{i(p+\ell)x\} = c_\ell\exp\{-((p+\ell)^2 - \omega^2)^{1/2}y\}\exp\{i(p+\ell)x\} \tag{2.14}$$

where $((p+\ell)^2 - \omega^2)^{1/2} > 0$. In the application to diffraction gratings terms of this type will be interpreted as surface waves.

$\underline{\omega = |p+\ell|}$. In this limiting case $\psi_\ell(y)$ is a linear combination of 1 and y and (2.5) implies that

$$\psi_\ell(y)\exp\{i(p+\ell)x\} = c_\ell\exp\{i(p+\ell)x\}\ . \tag{2.15}$$

Physically, (2.15) describes a plane wave that propagates parallel to the grating; i.e., a grazing wave. These waves divide the plane waves (2.12) from the surface waves (2.14). The frequencies $\{\omega = |p+\ell| \mid \ell \in Z\}$ are called the cut-off frequencies for R-B waves with x-momentum p.

An R-B wave ψ for G (for A) which satisfies the additional conditions

$$(2.16) \qquad c_\ell^- = 0 \text{ (resp. } c_\ell^+ = 0\text{) for all } \ell \text{ such that } \omega > |p + \ell|$$

will be said to be an outgoing (resp., incoming) R-B wave for G (for A). If

$$(2.17) \qquad c_\ell^- = c_\ell^+ = 0 \text{ for all } \ell \text{ such that } \omega > |p + \ell|$$

then ψ will be said to be an R-B surface wave for G (for A). Of course an R-B surface wave for A is both an outgoing and an incoming R-B wave for A. It is interesting that these are the only outgoing or incoming R-B waves for A. This is a consequence of

<u>Theorem 2.1</u>. Every outgoing (resp., incoming) R-B wave for A is an R-B surface wave for A.

A proof of this result has been given by Alber [3] in the case where ∂G is a curve of class C^2. The method is to apply Green's theorem to the R-B wave ψ for A and its conjugate in the region $G \cap \{X \mid -\pi < x < \pi,\ y < R\}$. In the case of an outgoing R-B wave for A this yields the equation

$$(2.18) \qquad \sum_{\omega > |p+\ell|} (\omega^2 - (p + \ell)^2)^{1/2} \, |c_\ell^+|^2 = 0$$

which implies that $c_\ell^+ = 0$ when $\omega > |p + \ell|$. For general grating domains the application of Green's theorem must be based on the generalized boundary conditions, as in [34, p. 57].

It will be seen in §4 that diffraction gratings may indeed support R-B surface waves and the question arises whether geometric criteria for the non-existence of such waves can be found. In the case of the Dirichlet boundary condition such a criterion was found by Alber [3] by adapting a method of F. Rellich [24] and D. M. Eidus [12]. Specialized to the grating domains considered here, Alber's theorem implies

Theorem 2.2. Let

$$G = \{X \mid y > h(x) \text{ for all } x \in R\} \tag{2.19}$$

where $h \in C^2(R)$ and $h(x + 2\pi) = h(x)$ for all $x \in R$. Then $A^D(G)$ has no R-B surface waves.

Theorem 2.1 implies that R-B waves for A may be determined, modulo R-B surface waves, by specifying either the coefficients c_ℓ^- with $\omega > |p + \ell|$ (the incoming plane waves) or the coefficients c_ℓ^+ with $\omega > |p + \ell|$ (the outgoing plane waves). R-B waves for A that contain a single incoming or outgoing plane wave will be used in the R-B wave expansions given in §6 below. These are the grating waves originally introduced by Rayleigh. Physically, they are the wave fields produced when the grating is illuminated by a single plane wave. Here they will be called R-B diffracted plane wave eigenfunctions for A or, for brevity, R-B wave eigenfunctions for A. There are two families determined by the presence of a single incoming and outgoing plane wave, respectively. The plane waves $\psi^{inc}(X,p,q)$ and $\psi^{inc}(X,p,-q)$ defined by (2.1) are incoming and outgoing R-B waves, respectively, with x-momentum p and frequency

$$\omega = \omega(p,q) = (p^2 + q^2)^{1/2} \quad . \tag{2.20}$$

The scattering of these waves by a grating will produce outgoing (resp., incoming) R-B waves with the same x-momentum and frequency. Hence the R-B wave eigenfunctions may be defined as follows.

Definition. The outgoing R-B diffracted plane wave for A with momentum $(p,q) \in R_0^2$ is a function $\psi_+(X,p,q)$ such that

(2.21) $\psi_+(\cdot,p,q)$ is an R-B wave for A, and

$$\psi_+(X,p,q) = \psi^{inc}(X,p,q) + \psi_+^{sc}(X,p,q) \tag{2.22}$$

where ψ_+^{sc} is an outgoing R-B wave for G. Similarly, the incoming R-B diffracted plane wave for A with momentum $(p,q) \in R_0^2$ is a function $\psi_-(X,p,q)$ such that

(2.23) $\psi_-(\cdot,p,q)$ is an R-B wave for A, and

$$\psi_-(X,p,q) = \psi^{inc}(X,p,-q) + \psi_-^{sc}(X,p,q) \tag{2.24}$$

where ψ_-^{sc} is an incoming R-B wave for G.

The uniqueness of $\psi_\pm(X,p,q)$ modulo R-B surface waves follows from Theorem 2.1, as was remarked above. Their existence for the class of gratings defined in §1 is proved in §6. Note also that the defining properties imply that

$$\psi_-(X,p,q) = \overline{\psi_+(X,-p,q)} \quad . \tag{2.25}$$

Hence the existence of the family ψ_- follows from that of ψ_+.

In the half-plane R_h^2 above the grating the R-B waves $\psi_\pm$ have Fourier expansions (2.10). For the function ψ_+ the expansion has the form

$$\psi_+(x,y,p,q) = (2\pi)^{-1} \exp\{i(px - qy)\}$$

$$(2.26) \qquad + \sum_{(p+\ell)^2<p^2+q^2} c_\ell^+(p,q) \exp\{i(p_\ell x + q_\ell y)\}$$

$$+ \sum_{(p+\ell)^2\geq p^2+q^2} c_\ell^+(p,q) \exp\{ip_\ell x\} \exp\{-((p+\ell)^2 - p^2 - q^2)^{1/2}\, y\}$$

where

$$(2.27) \qquad (p_\ell, q_\ell) = (p + \ell, \{p^2 + q^2 - (p + \ell)^2\}^{1/2}) \in R_0^2$$

defines the momentum of the reflected plane wave of order ℓ. Similarly,

$$\psi_-(x,y,p,q) = (2\pi)^{-1} \exp\{i(px + qy)\}$$

$$(2.28) \qquad + \sum_{(p+\ell)^2<p^2+q^2} c_\ell^-(p,q) \exp\{i(p_\ell x - q_\ell y)\}$$

$$+ \sum_{(p+\ell)^2\geq p^2+q^2} c_\ell^-(p,q) \exp\{ip_\ell x\} \exp\{-((p+\ell)^2 - p^2 - q^2)^{1/2}\, y\}$$

The relation (2.25) implies that the coefficients $c_\ell^\pm(p,q)$ in (2.26), (2.28) satisfy

$$(2.29) \qquad c_\ell^-(p,q) = \overline{c_{-\ell}^+(-p,q)} \quad \text{for all } (p,q) \in R_0^2 \text{ and } \ell \in Z .$$

The surface wave terms in (2.26) and (2.28) are exponentially decreasing functions of y except when the wave frequency $\omega(p,q) = (p^2 + q^2)^{1/2} = |p + \ell|$ for some $\ell \in Z$. These are precisely the cut-off frequencies mentioned above. In momentum space they form the exceptional set

$$(2.30) \qquad E = R_0^2 \cap \bigcup_{\ell \in Z} \{(p,q) \mid \sqrt{p^2 + q^2} = |p + \ell|\}$$

E is a set of confocal parabolas with foci at (0,0), axes along the p-axis and directrices $p + \ell = 0$, $\ell \in Z$. Two members of the family with directrices $p + \ell = 0$, $p + m = 0$ are disjoint if ℓ and m have the same sign and intersect orthogonally if ℓ and m have opposite signs. The family E thus divides R_0^2 into a system of curvilinear rectangles.

In the special case of the degenerate grating R_0^2 comparison of (1.33), (1.34) with (2.26), (2.28) shows that for the Neumann case $\psi_0^N = \psi_+ = \psi_-$, $c_0^{\pm}(p,q) = (2\pi)^{-1}$ and all other $c_\ell^{\pm}(p,q) = 0$. Similarly, for the Dirichlet case $\psi_0^D = i\psi_+ = -i\psi_-$, $c_0^{\pm}(p,q) = -(2\pi)^{-1}$ and all others $c_\ell^{\pm}(p,q) = 0$. Thus in these cases there is no scattering into higher order grating modes or surface waves, as was to be expected. Note that the defining properties (2.22), (2.24) can be rewritten as

$$(2.31) \qquad \psi_{\pm}(X,p,q) = \psi_0(X,p,q) + \psi'_{\pm}(X,p,q)$$

where ψ_0 is defined as at the end of §1 and ψ'_+ and ψ'_- are, respectively, outgoing and incoming R-B waves for G. This decomposition exhibits the R-B wave eigenfunctions for G as perturbations of those for R_0^2. The decomposition is used below for the construction of $\psi_{\pm}$ and the derivation of the eigenfunction expansions.

§3. The Reduced Grating Propagator A_p.

The quasi-periodicity property (2.3) of the R-B waves implies that they are completely determined by their values in the domain

$$\Omega = G \cap \{X \mid -\pi < x < \pi\} \ . \tag{3.1}$$

Moreover, (2.3) and the equation obtained from it by x-differentiation define boundary conditions that must be satisfied by R-B waves on the portions of $\partial\Omega$ where $x = \pm\pi$. These observations are used below to show that the R-B surface waves and diffracted plane waves for G are eigenfunctions and generalized eigenfunctions, respectively, of a p-dependent selfadjoint realization of $-\Delta$ in $L_2(\Omega)$. This operator, which will be denoted by A_p and called the reduced grating propagator, provides a basis for the construction of the R-B waves for G.

The definition of the grating domains in §1 implies that the reduced grating domains Ω satisfy

$$B_h \subset \Omega \subset B_0 \text{ for some } h > 0 \tag{3.2}$$

where

$$B_c = R_c^2 \cap \{X \mid -\pi < x < \pi\} = \{X \mid -\pi < x < \pi,\ y > c\} \ . \tag{3.3}$$

The notation

$$\gamma = \{y \mid (\pi,y) \in G\} = \{y \mid (-\pi,y) \in G\} \tag{3.4}$$

will also be used. The definition of the reduced grating propagators $A_p^N(\Omega)$ and $A_p^D(\Omega)$ associated with Ω and the two boundary conditions will be based on the function space

$$(3.5) \qquad L_2^{1,p}(\Omega) = L_2^1(\Omega) \cap \{u \mid u(\pi,y) = \exp\{2\pi i p\}\, u(-\pi,y),\ y \in \gamma\}$$

Sobolev's imbedding theorem [1] implies that every $u \in L_2^1(\Omega)$ has boundary values $u(\pm\pi,y)$ in $L_2^{\ell oc}(\gamma)$ and $L_2^{1,p}(\Omega)$ is a closed subspace of $L_2^1(\Omega)$.

The operator $A_p^N(\Omega)$ is defined by

$$(3.6) \qquad \begin{aligned} D(A_p^N(\Omega)) &= L_2^{1,p}(\Omega) \cap L_2^1(\Delta,\Omega) \\ &\cap \{u \mid \int_\Omega \{(\Delta u)\overline{v} + \nabla u \cdot \nabla\overline{v}\}\, dX = 0 \text{ for } v \in L_2^{1,p}(\Omega)\} \end{aligned}$$

and $A_p^N(\Omega)u = -\Delta u$. It can be shown that $A_p^N(\Omega)$ is the selfadjoint non-negative operator in $L_2(\Omega)$ associated via Kato's theory with the sesquilinear form defined by the Dirichlet integral acting on the domain $L_2^{1,p}(\Omega)$. By applying elliptic regularity theory [1] and Sobolev's imbedding theorem it can also be shown that every $u \in D(A_p^N(\Omega))$ satisfies the p-periodic boundary conditions

$$(3.7) \qquad \begin{cases} u(\pi,y) = \exp\{2\pi i p\}\, u(-\pi,y), & y \in \gamma \\ D_1 u(\pi,y) = \exp\{2\pi i p\}\, D_1 u(-\pi,y), & y \in \gamma \end{cases}$$

Moreover, if ∂G is a smooth curve then it follows from (1.14) as in §1 that functions $u \in D(A_p^N(\Omega))$ satisfy the Neumann boundary condition on

$$(3.8) \qquad \Gamma = \partial G \cap \overline{\Omega}$$

where $\overline{\Omega}$ is the closure of Ω in R^2.

To define $A_p^D(\Omega)$ several additional function spaces are needed. The subset of $C^\infty(G)$ consisting of functions that satisfy

$$(3.9) \qquad \phi(x + 2\pi,y) = \exp\{2\pi i p\}\, \phi(x,y) \text{ for all } (x,y) \in G$$

$$\text{(3.10)} \qquad \operatorname{supp} \phi \subset G \cap \{X \mid y < \rho\} \text{ where } \rho = \rho(\phi), \text{ and}$$

$$\text{(3.11)} \qquad \operatorname{dist}(\operatorname{supp} \phi, \partial G) > 0 \ ,$$

will be denoted by $C_p^\infty(G)$:

$$\text{(3.12)} \qquad C_p^\infty(G) = C^\infty(G) \cap \{\phi \mid (3.9), (3.10) \text{ and } (3.11) \text{ hold}\} \ .$$

The restrictions of such functions to Ω defines

$$\text{(3.13)} \qquad C_p^\infty(\Omega) = \{\psi = \phi|_\Omega \mid \phi \in C_p^\infty(G)\}$$

Finally,

$$\text{(3.14)} \qquad L_2^{D,p}(\Omega) = \text{Closure in } L_2^1(\Omega) \text{ of } C_p^\infty(\Omega) \ .$$

The operator $A_p^D(\Omega)$ is defined by

$$\text{(3.15)} \qquad \begin{aligned} &D(A_p^D(\Omega)) \\ &= L_2^{D,p}(\Omega) \cap L_2^1(\Delta,\Omega) \cap \{u \mid \int_\Omega \{(\Delta u)\bar{v} + \nabla u \cdot \overline{\nabla v}\}\, dX = 0 \text{ for } v \in L_2^{D,p}(\Omega)\} \end{aligned}$$

and $A_p^D(\Omega)u = -\Delta u$. In this case it can be shown that $A_p^D(\Omega)$ is the self-adjoint non-negative operator associated via Kato's theory with the sesquilinear form defined by the Dirichlet integral acting on the domain $L_2^{D,p}(\Omega)$. Again, functions in $D(A_p^D(\Omega))$ satisfy the p-periodic boundary conditions (3.7). Moreover, if ∂G is a smooth curve then functions $u \in D(A_p^D(\Omega))$ satisfy the Dirichlet boundary condition on Γ.

The operators $A_p^N(\Omega)$ and $A_p^N(\Omega)$ will be shown in §4 to have continuous spectra. To define corresponding generalized eigenfunctions it will be convenient to define extensions of $A_p^N(\Omega)$ and $A_p^D(\Omega)$ in $L_2^{\ell oc}(\Omega)$. The following subsets of $L_2^{\ell oc}(\Omega)$ are also needed:

$$(3.16)\qquad L_2^{1,p,\ell oc}(\Omega) = L_2^{1,\ell oc}(\Omega) \cap \{u \mid u(\pi,y) = \exp\{2\pi i p\}\, u(-\pi,y),\ y \in \gamma\}\ ,$$

$$(3.17)\qquad L_2^{D,p,\ell oc}(\Omega) = \text{Closure of } C_p^{\infty}(\Omega) \text{ in } L_2^{1,\ell oc}(\Omega)\ .$$

Each is a closed subspace of the Fréchet space $L_2^{1,\ell oc}(\Omega)$. The sets

$$(3.18)\qquad \begin{cases} L_2^{1,p,com}(\Omega) = L_2^{1,p}(\Omega) \cap L_2^{com}(\Omega) \\ L_2^{D,p,com}(\Omega) = L_2^{D,p}(\Omega) \cap L_2^{com}(\Omega) \end{cases}$$

will also be used.

The operator $A_p^{N,\ell oc}(\Omega)$ is the extension of $A_p^N(\Omega)$ in $L_2^{\ell oc}(\Omega)$ defined by

$$(3.19)\qquad \begin{aligned} D(A_p^{N,\ell oc}(\Omega)) &= L_2^{1,p,\ell oc}(\Omega) \cap L_2^{1,\ell oc}(\Delta,\Omega) \\ &\cap \{u \mid \int_\Omega \{(\Delta u)\overline{v} + \nabla u \cdot \nabla \overline{v}\}\, dX = 0 \text{ for } v \in L_2^{1,p,com}(\Omega)\} \end{aligned}$$

and $A_p^{N,\ell oc}(\Omega)u = -\Delta u$. Similarly, $A_p^{D,\ell oc}(\Omega)$ is the extension of $A_p^D(\Omega)$ in $L_2^{\ell oc}(\Omega)$ defined by

$$(3.20)\qquad \begin{aligned} D(A_p^{D,\ell oc}(\Omega)) &= L_2^{D,p,\ell oc}(\Omega) \cap L_2^{1,\ell oc}(\Delta,\Omega) \\ &\cap \{u \mid \int_\Omega \{(\Delta u)\overline{v} + \nabla u \cdot \nabla \overline{v}\}\, dX = 0 \text{ for } v \in L_2^{D,p,com}(\Omega)\} \end{aligned}$$

and $A_p^{D,\ell oc}(\Omega)u = -\Delta u$. It is easy to verify that $D(A_p^{N,\ell oc}(\Omega))$ and $D(A_p^{D,\ell oc}(\Omega))$ are closed linear subspaces of the Fréchet space $L_2^{1,\ell oc}(\Delta,\Omega)$ and hence are themselves Fréchet spaces.

The reduced grating propagators for the degenerate grating will be denoted by

$$(3.21)\qquad A^N_{0,p} = A^N_p(B_0), \quad A^D_{0,p} = A^D_p(B_0), \text{ and}$$

$$(3.22)\qquad A^{N,\ell oc}_{0,p} = A^{N,\ell oc}_p(B_0),\ A^{D,\ell oc}_{0,p} = A^{D,\ell oc}_p(B_0) .$$

Moreover, the condensed notation of §1 will be used; i.e., A_p will be used to denote either $A^N_p(\Omega)$ *or* $A^D_p(\Omega)$ in stating results valid for both. Similarly, $A^{\ell oc}_p$ will be used to denote $A^{N,\ell oc}_p(\Omega)$ or $A^{D,\ell oc}_p(\Omega)$. In particular, for the degenerate grating the notation $A_{0,p}$ is used for $A^N_{0,p}$ and $A^D_{0,p}$ and $A^{\ell oc}_{0,p}$ is used for $A^{N,\ell oc}_{0,p}$ and $A^{D,\ell oc}_{0,p}$.

Note that all the p-dependent function spaces defined above are periodic functions of p with period 1. It follows that

$$(3.23)\qquad A_{p+m} = A_p,\ A^{\ell oc}_{p+m} = A^{\ell oc}_p \text{ for all } m \in Z .$$

Hence it will suffice to study A_p and $A^{\ell oc}_p$ for the reduced momenta $p \in (-1/2,1/2]$.

The resolvent set and spectrum of A_p will be denoted by $\rho(A_p)$ and $\sigma(A_p)$ respectively. Clearly $\sigma(A_p) \subset [0,\infty)$ since A_p is selfadjoint and non-negative. In fact, it will be shown that

$$(3.24)\qquad \sigma(A_p) = [p^2,\infty) \text{ for all } p \in (-1/2,1/2] .$$

This was proved directly by Alber in the cases considered by him [3]. Here it follows from the eigenfunction expansions for A_p given in §5. $\sigma(A_p)$ is a continuous spectrum which, in general, will have embedded eigenvalues. It will be shown in §4 that $\sigma_0(A_p)$, the point spectrum of A_p, is discrete; that is, each interval contains finitely many eigenvalues of A_p and the eigenvalues have finite multiplicity. It is of interest for the applications to diffraction gratings to have criteria for $\sigma_0(A_p)$ to be empty. While completely general criteria are not known it will be shown that the hypotheses of Theorem 2.2 imply $\sigma_0(A_p^D) = \phi$ for all $p \in (-1/2,1/2]$.

Eigenfunction expansions for A_p are derived in §5 by perturbation theory starting from $A_{0,p}$. The expansions for $A_{0,p}$, which are elementary, are recorded here as a starting point for the analysis of A_p. Separation of variables applied to $A_{0,p}^N$ leads to the complete family of generalized eigenfunctions

$$\phi_0^N(X,p+m,q) = \frac{1}{\pi} e^{i(p+m)\cdot x} \cos qy,\ m \in Z,\ q > 0 \tag{3.25}$$

where $p \in (-1/2,1/2]$ is fixed. Similarly, for $A_{0,p}^D$ one finds the complete family

$$\phi_0^D(X,p+m,q) = \frac{1}{\pi} e^{i(p+m)\cdot x} \sin qy,\ m \in Z,\ q > 0\ . \tag{3.26}$$

To describe the eigenfunction expansions for $A_{0,p}$ the condensed notation $\phi_0(X,p+m,q)$ will be used to denote either ϕ_0^N or ϕ_0^D. Note that

$$\phi_0(X,p+m,q) = \psi_0(X,p+m,q)\big|_{B_0}\ , \tag{3.27}$$

that is, the generalized eigenfunctions for $A_{0,p}$ are obtained from those of A_0 by restricting X to B_0 and the x-momentum parameter to the lines $p' = p + m$ with $m \in Z$ and $p \in (-1/2,1/2]$ fixed. Classical Plancherel theory implies that if $R_0 = (0,\infty)$ then for all $f \in L_2(B_0)$ the limits

$$\tilde{f}_0(p+m,q) = L_2(R_0)\text{-}\lim_{M\to\infty} \int_{B_0,} \overline{\phi_0(X,p+m,q)}\, f(X)\, dX \tag{3.28}$$

exist for $m \in Z$ and $p \in (-1/2,1/2]$ fixed, where $B_{0,M} = B_0 \cap \{X \mid y < M\}$. Note that the $L_2(R_0)$-convergence refers to the variable q. Moreover, Parseval's formula holds in the form

$$\|f\|^2_{L_2(B_0)} = \sum_{m\in Z} \|\tilde{f}_0(p+m,\cdot)\|^2_{L_2(R_0)} \tag{3.29}$$

Hence, the sequence

$$\{\tilde{f}_0(p+m,\cdot) \in L_2(R_0) \mid m \in Z\} \in \sum_{m\in Z} \oplus L_2(R_0) \tag{3.30}$$

and the operator $\Phi_{0,p}\colon L_2(B_0) \to \sum_{m\in Z} \oplus L_2(R_0)$, defined by

$$\Phi_{0,p} f = \{\tilde{f}_0(p+m,\cdot) \mid m \in Z\}, \tag{3.31}$$

is an isometry. A more careful application of the Plancherel theory shows that $\Phi_{0,p}$ is unitary. Finally, calculation of the spectral family $\{\Pi_{0,p}(\mu) \mid \mu \geq p^2\}$ for $A_{0,p}$ gives

$$\Pi_{0,p}(\mu)\, f(X) = \sum_{(p+m)^2\leq\mu} \int_0^{(\mu-(p+m)^2)^{1/2}} \phi_0(X,p+m,q)\, \tilde{f}_0(p+m,q)\, dq \tag{3.32}$$

In particular, making $\mu \to \infty$ gives the eigenfunction expansion

$$f(X) = L_2(B_0)\text{-}\lim_{M\to\infty} \sum_{|m|\leq M} \int_0^M \phi_0(X,p+m,q)\, \tilde{f}_0(p+m,q)\, dq . \tag{3.33}$$

The relationship between the R-B waves for A and the reduced propagators A_p will now be discussed. Note first that if ψ is an R-B surface wave for A with x-momentum $p + m$ $(-1/2 < p \leq 1/2,\ m \in Z)$ and $\omega \notin \{|p + \ell| \mid \ell \in Z\}$ then $\psi \in D(A^{\ell oc})$ and for $y > h$

$$(3.34) \qquad \psi(x,y) = \sum_{|p+\ell|>\omega} c_\ell \exp\{i(p+\ell)x\} \exp\{-((p+\ell)^2-\omega^2)^{1/2} y\} .$$

It follows that $\phi(x,y) = \psi(x,y)|_\Omega \in D(A_p)$ and $A_p\phi = \omega^2\phi$. Thus ϕ is an eigenfunction of A_p. To formulate the converse, note that every $\phi \in L_2^{\ell oc}(\Omega)$ has a unique p-periodic extension $\psi \in L_2^{\ell oc}(G)$. It is easy to verify that if

$$(3.35) \qquad \Omega^{(m)} = \Omega + (2\pi m, 0)$$

then for each $m \in Z$ the extension ψ is given by

$$(3.36) \qquad \psi(x,y) = \exp\{2\pi imp\}\, \phi(x-2\pi m, y) \text{ for all } (x,y) \in \Omega^{(m)} .$$

This defines ψ in $L_2^{\ell oc}(G)$ because G differs from $\bigcup_{m\in Z} \Omega^{(m)}$ by a Lebesgue null set. The operator $\mathcal{O}^p$: $L_2^{\ell oc}(\Omega) \to L_2^{\ell oc}(G)$ defined by (3.36) maps $L_2^{\ell oc}(\Omega)$ one-to-one onto the set of all p-periodic functions in $L_2^{\ell oc}(G)$. With this notation it is not difficult to show that if ϕ is an eigenfunction of A_p then $\psi = \mathcal{O}^p\phi$ is an R-B surface wave for A with reduced x-momentum p.

The relationship between R-B diffracted plane waves for A and generalized eigenfunctions of A_p is exemplified by (3.27). More generally, if $\psi(X,p+m,q)$ is an R-B diffracted plane wave for A with $-1/2 < p \le 1/2$, $m \in Z$ then $\phi_\pm(X,p+m,q) = \psi_\pm(X,p+m,q)|_\Omega$ satisfies $\phi_\pm(\cdot,p+m,q) \in D(A_p^{\ell oc})$, $(\Delta + \omega^2(p+m,q))\, \phi_\pm(X,p+m,q) = 0$ in Ω and

$$(3.37) \qquad \phi_\pm(X,p+m,q) = \phi_0(X,p+m,q) + \phi'_\pm(X,p+m,q),\ y \ge h,$$

where ϕ'_+ (resp., ϕ'_-) has a Fourier expansion that contains only outgoing (resp., incoming) plane waves and exponentially damped waves. Functions

$\phi_+(X,p+m,q)$ and $\phi_-(X,p+m,q)$ with these properties will be called, respectively, outgoing and incoming diffracted plane waves for A_p. They are unique modulo eigenfunctions of A_p. It is now easy to verify that if $\phi_+(X,p+m,q)$ (resp., $\phi_-(X,p+m,q)$) is an outgoing (resp., incoming) diffracted plane wave for A_p then $\psi_+(X,p+m,q) = \mathcal{O}^p\ \phi_+(X,p+m,q)$ (resp., $\psi_-(X,p+m,q) = \mathcal{O}^p\ \phi_-(X,p+m,q)$) is an outgoing (resp., incoming) R-B diffracted plane wave for A with x-momentum $p + m$. These relationships will be used in §6 to construct the R-B diffracted plane waves for A.

§4. Analytic Continuation of the Resolvent of A_p.

An analytic continuation of the resolvent

$$R(A_p,z) = (A_p - z)^{-1} \tag{4.1}$$

across the spectrum $\sigma(A_p) = [p^2,\infty)$ is constructed in this section by an elegant and powerful method that was introduced into scattering theory by H. D. Alber [3]. The continuation provides the basis for the construction in §5 of the diffracted plane waves $\phi_\pm(X,p,q)$ for A_p and the derivation of the corresponding eigenfunction expansions.

For each pair of extended real numbers r,r' satisfying $0 \le r < r' \le +\infty$ let

$$\begin{aligned} B_{r,r'} &= \{X \mid -\pi < x < \pi,\ r < y < r'\}\ ,\quad B_r = B_{r,\infty}\ , \\ \Omega_{r,r'} &= \Omega \cap B_{r,r'}\ ,\quad \Omega_r = \Omega_{r,\infty}\ . \end{aligned} \tag{4.2}$$

Moreover, let $P_r : L_2(\Omega_{0,r}) \to L_2(\Omega)$ denote the linear operator defined by

$$P_r\, u(X) = \begin{cases} u(X)\ , & X \in \Omega_{0,r} \\ 0\ , & X \in \Omega_r\ . \end{cases} \tag{4.3}$$

The goal of §4 may be formulated with this notation. It is to construct an analytic continuation of

$$z \to R(A_p,z)\, P_r : L_2(\Omega_{0,r}) \to L_2^{\ell oc}(\Omega) \tag{4.4}$$

from the resolvent set $\rho(A_p) = C - [p^2,\infty)$ across $\sigma(A_p) = [p^2,\infty)$. For this purpose $\rho(A_p)$ will be embedded in a Riemann surface M_p.

The definition of M_p may be motivated by considering the linear space of functions

$$(4.5) \qquad E_{p,z,r} = D(A_p^{\ell oc}) \cap \{u \mid \operatorname{supp}\,(\Delta + z)u \subset \Omega_{0,r}\}\ , \quad r > h\ .$$

Basic properties of $E_{p,z,r}$ are described by

Lemma 4.1. Every $u \in E_{p,z,r}$ satisfies

$$(4.6) \qquad u \in L_2^{2,\ell oc}(\Omega_h)$$

$$(4.7) \qquad u(x,y) = \sum_{m\in Z} u_m(y)\, e^{i(p+m)x} \text{ in } \Omega_h$$

where the series converges in $L_2^{2,\ell oc}(\Omega_h)$,

$$(4.8) \qquad u_m(y) \in L_2^{2,\ell oc}(R_h)\ , \quad R_h = (h,\infty)\ .$$

Moreover, if $\overline{\Omega}_r$ denotes the closure of Ω_r in R^2,

$$(4.9) \qquad u \in C^\infty(\overline{\Omega}_r)\ , \text{ and}$$

$$(4.10) \qquad u_m(y) = c_m^+ \exp\{iy(z-(p+m)^2)^{1/2}\} + c_m^- \exp\{-iy(z-(p+m)^2)^{1/2}\}$$

for $y \geq h$ where $c_m^\pm$ are constants and

$$(4.11) \qquad \operatorname{Im}\,(z - (p+m)^2)^{1/2} \geq 0\ .$$

Properties (4.6) and (4.9) follow from elliptic regularity theory [1], while (4.7) and (4.8) follow from classical Fourier theory. The convergence of (4.7) in $L_2^{2,\ell oc}(\Omega_h)$ follows from the fact that the partial sums of the Fourier series define orthogonal projections in $L_2^2(\Omega_{r,r'})$ for $h \leq r < r' < \infty$. (4.10) follows from (4.9) and the equation $\Delta u + zu = 0$ in Ω_r.

Note that if $z \in \rho(A_p)$ and $u = R(A_p,z)P_r f$ with $f \in L_2(\Omega_{0,r})$ then $u \in L_2(\Omega) \cap \mathcal{E}_{p,z,r}$ and hence $c_m^- = 0$ for all m and $c_m^+ = 0$ when $\operatorname{Im}(z - (p + m)^2)^{1/2} = 0$. This suggests that M_p be defined as the Riemann surface associated with the family of holomorphic functions on $C - [p^2,\infty)$ defined by

(4.12) $$\{z \to (z - (p+m)^2)^{1/2} \mid \operatorname{Im}(z - (p+m)^2)^{1/2} > 0 \text{ for all } m \in Z\} .$$

M_p is uniquely determined up to isomorphism by the following three properties [3, 21]:

(4.13) M_p is connected and every function of the family (4.12) can be continued analytically to all of M_p.

(4.14) For every pair of points of M_p that lie over the same point of C there are at least two functions of the family that take different values at these points.

(4.15) M_p is maximal with respect to these two properties.

The following notation will be used in connection with M_p. ζ will denote a generic point of M_p and $\pi = \pi_p : M_p \to C$ will denote the canonical projection of M_p onto C. The subscript p will be omitted when there is no danger of ambiguity. The analytic continuation of $(z - (p + m)^2)^{1/2}$ from $C - [p^2,\infty)$ to M_p will be denoted by $w_{p+m}(\zeta)$. Thus, for all $\zeta \in M_p$,

(4.16) $$w_{p+m}(\zeta) = \pm(\pi(\zeta) - (p + m)^2)^{1/2} .$$

M_p^+ will denote that component of M_p over $C - [p^2,\infty)$ on which

Im $w_{p+m}(\zeta) > 0$ for all $m \in Z$. Finally, $T_p = \{(p+m)^2 \mid m \in Z\} \subset C$ will denote the set of branch points of the family (4.12).

The properties of M_p include the following. M_p has infinitely many sheets. More precisely, for each disk $D(z_0,\rho) \subset C$, $\pi^{-1}(D(z_0,\rho))$ has infinitely many components. If $z_0 = (p+m)^2$ for some $m \in Z$ then the set $\pi^{-1}(D(z_0,\rho))$ contains infinitely many branch points. Moreover, for all $\zeta \in M_p$ the set $\{m \mid \text{Im } w_{p+m}(\zeta) \leq 0\}$ is finite [3]. Finally, $M_{p+m} = M_p$ for all $m \in Z$.

In addition to M_p the set

$$(4.17) \qquad M = \bigcup_{-1/2<p\leq 1/2} \{(p,\zeta) \mid \zeta \in M_p\}$$

will be needed to describe the dependence of the continuation of $R(A_p,\pi(\zeta))P_r$ on p and ζ. M will be topologized in such a way that each function $(p,\zeta) \to w_{p+m}(\zeta)$, $m \in Z$, is continuous on M. To this end let $(p_0,\zeta_0) \in M$ and define

$$(4.18) \qquad z_0 = \pi_{p_0}(\zeta_0)\ , \ D(z_0,\rho) = \{z \mid |z - z_0| < \rho\}$$

and

$$(4.19) \qquad U(p_0,\zeta_0,\rho) = \text{Component of } \pi_{p_0}^{-1}(D(z_0,\rho)) \text{ containing } \zeta_0 \ (\subset M_{p_0})$$

To define a neighborhood basis for M at (p_0,ζ_0) three cases will be distinguished.

<u>Case 1</u>. $z_0 \notin [p_0^2,\infty)$. If $\rho_0 > 0$ is the distance from z_0 to $[p_0^2,\infty)$ then for $\rho < \rho_0$ $D(z_0,\rho) \cap [p_0^2,\infty) = \phi$ and $U(p_0,\zeta_0,\rho)$ contains no branch points of M_{p_0}. In this case

(4.20) $\{\operatorname{sgn} \operatorname{Im} w_{p_0+m}(\zeta) \mid m \in Z\}$, $\zeta \in U(p_0,\zeta_0,\rho)$

is well defined. Moreover, $|p - p_0| < \delta$ implies that $D(z_0,\rho) \cap [p^2,\infty) = \phi$ for δ small enough and hence $\{\operatorname{sgn} \operatorname{Im} w_{p+m}(\zeta) \mid m \in Z\}$ is also well defined on the components of $\pi_p^{-1}(D(z_0,\rho))$. In this case one may define $U(p,\zeta_0,\rho)$ as the component of $\pi_p^{-1}(D(z_0,\rho))$ for which

(4.21) $\{\operatorname{sgn} \operatorname{Im} w_{p+m}(\pi_p^{-1}(z)) \mid m \in Z\} = \{\operatorname{sgn} \operatorname{Im} w_{p_0+m}(\pi_{p_0}^{-1}(z)) \mid m \in Z\}$

for $z \in D(z_0,\rho)$. A corresponding neighborhood of (p_0,ζ_0) in M is defined by

(4.22) $$N(p_0,\zeta_0,\rho,\delta) = \bigcup_{|p-p_0|<\delta} \{(p,\zeta) \mid \zeta \in U(p,\zeta_0,\rho)\} .$$

Case 2. $z_0 \in [p_0^2,\infty) - T_{p_0}$. In this case if ρ_0 is the distance from z_0 to the set T_{p_0} then for $\rho < \rho_0$ $U(p_0,\zeta_0,\rho)$ contains no branch points of M_{p_0} and (4.20) is well defined provided $\pi_{p_0}(\zeta) \in D_+(z_0,\rho) = D(z_0,\rho) \cap \{z \mid \operatorname{Im} z > 0\}$. Moreover, $|p - p_0| < \delta$ implies that $D(z_0,\rho)$ contains no points of T_p, for δ small enough, and hence $\{\operatorname{sgn} \operatorname{Im} w_{p+m}(\zeta) \mid m \in Z\}$ is also well defined if $\pi_p(\zeta) \in D_+(z_0,\rho)$. In this case one defines $U(p,\zeta_0,\rho)$ as the component of $\pi_p^{-1}(D(z_0,\rho))$ for which (4.21) holds for $z \in D_+(z_0,\rho))$. A corresponding neighborhood is again defined by (4.22).

Case 3. $z_0 = (p_0 + m_0)^2$ for some $m_0 \in Z$. If $\rho_0 > 0$ is the distance from z_0 to the set $T_{p_0} - \{(p_0 + m_0)^2\}$ then for $\rho < \rho_0$ the set $U(p_0,\zeta_0,\rho)$ contains only one branch point; namely, that for $w_{p_0+m_0}(\zeta)$. Hence $\{\operatorname{sgn} \operatorname{Im} w_{p_0+m}(\zeta) \mid m \in Z - \{m_0\}\}$ is well defined for $\zeta \in U(p_0,\zeta_0,\rho)$ and $\pi_{p_0}(\zeta) \in D_+(z_0,\rho)$. Moreover, $|p - p_0| < \delta$ implies that $D(z_0,\rho)$ contains $(p + m_0)^2$ and no other points of the set $\mathcal{T}_p$ and hence $\{\operatorname{sgn} \operatorname{Im} w_{p+m}(\zeta) \mid m \in Z - \{m_0\}\}$ is well defined on the components of $\pi_p^{-1}(D_+(z_0,\rho))$. In this case one may define $U(p,\zeta_0,\rho)$ as the component of $\pi_p^{-1}(D(z_0,\rho))$ for which

$$
\begin{aligned}
&\{\operatorname{sgn} \operatorname{Im} w_{p+m}(\pi_p^{-1}(z)) \mid m \in Z - \{m_0\}\} \\
&\qquad = \{\operatorname{sgn} \operatorname{Im} w_{p_0+m}(\pi_{p_0}^{-1}(z)) \mid m \in Z - \{m_0\}\}
\end{aligned}
\tag{4.23}
$$

for all $z \in D_+(z_0,\rho)$. A corresponding neighborhood is again defined by (4.22).

The topology of $\mathcal{M}$ is defined to be the one generated by the neighborhood bases defined above and one has

Theorem 4.2. Each of the functions on $\mathcal{M}$ defined by

$$
(p,\zeta) \to w_{p+m}(\zeta) \quad , \; m \in Z
\tag{4.24}
$$

is continuous on $\mathcal{M}$. Moreover, the family of functions $\{(p,\zeta) \to w_{p+m}(\zeta) \mid m \in Z\}$ is equicontinuous in $\mathcal{M}$.

The theorem that $\{\zeta \to w_{p+m}(\zeta) \mid m \in Z\}$ is equicontinuous on $\mathcal{M}_p$ for fixed p was proved by Alber [3]. Theorem 4.2 plays a key role in proving the continuity in (p,q) of the Rayleigh-Bloch waves in §6.

The Fréchet Space $\mathcal{F}_{p,\zeta,r}$. To describe the subset of $\mathcal{E}_{p,z,r}$ that contains the analytic continuation of $R(A_p,z)P_r f$ to $\mathcal{M}_p$, consider the set of functions $u \in \mathcal{E}_{p,z,r}$ whose Fourier representations (4.7), (4.10) in Ω_r satisfy

$$
\text{For each } m \in Z, \text{ either } c_m^+ = 0 \text{ or } c_m^- = 0, \text{ and}
\tag{4.25}
$$

$$
c_m^- = 0 \text{ for all but a finite number of } m \in Z .
\tag{4.26}
$$

Note that these conditions express the "radiation conditions"

$$(4.27)\qquad [D_y \pm i(z - (p+m)^2)^{1/2}]\, u_m(y) = 0 \;,\; y \geq r \;,$$

where for each m either "+" or "-" is chosen and "-" is chosen for all but a finite number of $m \in Z$. It is clear that each such $u \in E_{p,z,r}$ is associated with a unique point $\zeta \in M_p$ such that $\pi_p(\zeta) = z$ and the Fourier expansion (4.7), (4.10) of u has the form

$$(4.28)\qquad u(x,y) = \sum_{m\in Z} c_m \exp\{i(p+m)x + i\,y\,w_{p+m}(\zeta)\} \;,\; y \geq r \;.$$

For each $(p,\zeta) \in M$ and each $r > h$ the set of all such solutions will be denoted by

$$(4.29)\qquad F_{p,\zeta,r} = D(A_p^{\ell oc}) \cap \{u \mid \operatorname{supp}\, (\Delta + \pi_p(\zeta))u \subset \Omega_{0,r} \text{ and (4.28) holds}\} \;.$$

Note that $F_{p,\zeta,r} \subset D(A_p^{\ell oc}) \subset L_2^{1,\ell oc}(\Delta,\Omega)$ and recall that $D(A_p^{\ell oc})$ is closed in $L_2^{1,\ell oc}(\Delta,\Omega)$. This implies

<u>Theorem 4.3</u>. $F_{p,\zeta,r}$ is closed in $D(A_p^{\ell oc})$ in the topology of $L_2^{1,\ell oc}(\Delta,\Omega)$ and hence is a Fréchet space.

This is immediate because the defining properties of $F_{p,\zeta,r}$, namely supp $(\Delta + \pi_p(\zeta))u \subset \Omega_{0,r}$ and $[D_y - i\, w_{p+m}(\zeta)]\, u_m = 0$ in $y \geq r$, are preserved under convergence in $L_2^{1,\ell oc}(\Delta,\Omega)$.

The following condensed notation will be used in discussing $F_{p,\zeta,r}$ and related operators:

$$(4.30)\qquad (u,v)_{r,r'} = (u,v)_{L_2(\Omega_{r,r'})} \;,$$

$$(4.31) \qquad (u,v)_{1;r,r'} = (u,v)_{L_2^1(\Omega_{r,r'})} ,$$

$$(4.32) \qquad (u,v)_{1;\Delta;r,r'} = (u,v)_{L_2^1(\Delta,\Omega_{r,r'})} .$$

Now let $P_{p,\zeta,r} : \mathcal{F}_{p,\zeta,r} \to L_2(\Omega_{0,r})$ denote the natural projection defined by

$$(4.33) \qquad P_{p,\zeta,r}\, u = u|_{\Omega_{0,r}} \text{ for all } u \in \mathcal{F}_{p,\zeta,r} .$$

An important property of $\mathcal{F}_{p,\zeta,r}$ is expressed by the following generalization of a theorem of Alber [3, p. 264].

Theorem 4.4. For every compact set $K \subset \mathcal{M}$ and for every $r' > r$ there exists a constant $C = C(K,r,r')$ such that

$$(4.34) \qquad \|u\|_{1;\Delta;0,r'} \le C\, \|P_{p,\zeta,r}\, u\|_{1;\Delta;0,r}$$

for all $u \in \bigcup_{(p,\zeta)\in K} \mathcal{F}_{p,\zeta,r}$. In particular, $P_{p,\zeta,r}$ is a topological isomorphism of $\mathcal{F}_{p,\zeta,r}$ onto $P_{p,\zeta,r}\, \mathcal{F}_{p,\zeta,r}$, topologized by the $L_2^1(\Delta,\Omega_{0,r})$-norm.

The Operators $A_{p,\zeta,r} : L_2(\Omega_{0,r}) \to L_2(\Omega_{0,r})$. Following Alber's program, the construction of the analytic continuation of $R(A_p,z)P_r$ to $\mathcal{M}_p$ will be based on the family of linear operators $A_{p,\zeta,r}$ in $L_2(\Omega_{0,r})$, defined for all $(p,\zeta) \in \mathcal{M}$ by

$$(4.35) \qquad D(A_{p,\zeta,r}) = P_{p,\zeta,r}\, \mathcal{F}_{p,\zeta,r} ,$$

$$(4.36) \qquad A_{p,\zeta,r}\, u = -\Delta u .$$

The properties of $A_{p,\zeta,r}$ that are fundamental for the analytic continuation of $R(A_p,z)$ are described by the following theorems.

Theorem 4.5. For every $(p,\zeta) \in M$ and every $r > h$ the operator $A_{p,\zeta,r}$ is m-sectorial in the sense of Kato [17, p. 279].

Theorem 4.6. For all grating domains of the class defined in §1, the family of operators $\{A_{p,\zeta,r} \mid (p,\zeta) \in M\}$ is continuous in the sense of generalized convergence (Kato [17, p. 206]). Moreover, for each fixed $p \in (-1/2,1/2]$ the family $\{A_{p,\zeta,r} \mid \zeta \in M_p\}$ is holomorphic in the generalized sense (Kato [17, p. 366]).

Theorem 4.7. For every $(p,\zeta) \in M$, every $r > h$ and every $z \in \rho(A_{p,\zeta,r})$ the resolvent $R(A_{p,\zeta,r},z) = (A_{p,\zeta,r} - z)^{-1}$ is a compact operator in $L_2(\Omega_{0,r})$ and hence $\sigma(A_{p,\zeta,r})$ is discrete.

Theorem 4.5 generalizes Alber [3, Th. 5.5]. As in [3] it may be proved by associating $A_{p,\zeta,r}$ with a densely defined, closed, sectorial sesquilinear form in $L_2(\Omega_{0,r})$ and using Kato's first representation theorem [17, p. 322]. The second statement of Theorem 4.6 generalizes Alber [3, Th. 5.5b]. The hypothesis $G \in S$ of §1 is needed to prove Theorem 4.6. Theorem 4.7, which generalizes Alber [3, Th. 5.5a], is a consequence of the local compactness property of G in the case of the Neumann boundary conditions. Complete proofs of Theorems 4.5, 4.6 and 4.7 are given in [38]. The following consequences of these theorems are needed for the spectral analyses of A_p and A in §§5-6.

Theorem 4.8. For all $\zeta \in M_p^+$ one has $\pi_p(\zeta) \in \rho(A_{p,\zeta,r})$ and

$$R(A_{p,\zeta,r},\pi_p(\zeta)) = P_{p,\zeta,r}\, R(A_p,\pi_p(\zeta))\, P_r \ . \tag{4.37}$$

This result may be verified by direct calculation.

Theorem 4.9. For every $p \in (-1/2,1/2]$ the set

$$\textstyle\sum_p = \{\zeta \mid \pi_p(\zeta) \in \sigma(A_{p,\zeta,r})\} \subset M_p \tag{4.38}$$

has no accumulation points in M_p and is independent of $r > h$.

This result, which generalizes [3, Th. 5.5c], is a consequence of Theorem 4.7. For brevity the resolvent of (4.37) will be denoted by

$$R_{p,\zeta,r} = R(A_{p,\zeta,r}, \pi_p(\zeta)) \in B(L_2(\Omega_{0,r})) \ . \tag{4.39}$$

Here B(X) denotes the bounded operators on X.

Corollary 4.10. For each $p \in (-1/2, 1/2]$ and $r > h$ the mapping

$$\zeta \to R_{p,\zeta,r} \in B(L_2(\Omega_{0,r})) \tag{4.40}$$

is finitely meromorphic on M_p with pole set Σ_p.

This result is based on a theorem of S. Steinberg [28]; cf. [3, Th. 5.5e]. Theorem 4.4 and 4.8 provide the analytic continuation of $R(A_p, z)\, P_r$ in the following form.

Corollary 4.11. The analytic continuation to M_p of

$$\zeta \to R(A_p, \pi_p(\zeta)) P_r \in B(L_2(\Omega_{0,r}) \ , \ L_2^{1,\ell oc}(\Delta,\Omega)) \ , \ \zeta \in M_p^+ \ , \tag{4.41}$$

is given by

$$\zeta \ \to P_{p,\zeta,r}^{-1} \ R_{p,\zeta,r} \in B(L_2(\Omega_{0,r}), \ L_2^{1,\ell oc}(\Delta,\Omega)), \ \zeta \in M_p \ , \tag{4.42}$$

where B(X,Y) denotes the bounded linear operators from X to Y.

Corollary 4.12. For all grating domains of the class defined in §1, the point spectrum $\sigma_0(A_p)$ is discrete.

This result follows from Theorem 4.9 and Corollary 4.10.

Corollary 4.13. For all grating domains of the class defined in §1 one has

$$\pi_p(\overline{M_p^+} \cap \Sigma_p) \subset \sigma_0(A_p) \cup T_p \tag{4.43}$$

where $\overline{M_p^+}$ is the closure of M_p^+ in M_p.

If $\sigma_0(A_p) = \phi$ then (4.43) means that the poles of $R_{p,\zeta,r}$ that lie above the spectrum $\sigma(A_p) = [p^2,\infty)$ must lie above the branch point set T_p. The fact that such poles may or may not occur is illustrated by the two operators A_0^D and A_0^N corresponding to the degenerate grating. For A_0^D, separation of variables leads to a construction of the Green's function (= kernel of the resolvent $R(A_0^D,z)$) which can be written

$$\begin{aligned} &G_0^D(X,X',p,z) \\ (4.44)\quad & \\ &= \frac{i}{2\pi} \sum_{m\in Z} e^{i(p+m)(x-x')}(z-(p+m)^2)^{-1/2}\sin(z-(p+m)^2)^{1/2}\, y_< \, e^{i(z-(p+m)^2)^{1/2}\, y_>} \end{aligned}$$

where $y_< = \mathrm{Min}\,(y,y')$, $y_> = \mathrm{Max}\,(y,y')$. The analogous calculation for A_0^N gives

$$\begin{aligned} &G_0^N(X,X',p,z) \\ (4.45)\quad & \\ &= \frac{i}{2\pi} \sum_{m\in Z} e^{i(p+m)(x-x')}(z-(p+m)^2)^{-1/2}\cos(z-(p+m)^2)^{1/2}\, y_< \, e^{i(z-(p+m)^2)^{1/2}\, y_>} . \end{aligned}$$

In the first case $R(A_0^D,z)$ has no poles for real $z = \lambda \pm i0 \in [p^2,\infty)$. In the second case $R(A_0^N,z)$ has a simple pole at each of the points $z = \lambda \pm i0 \in T_p$.

The following two theorems are implied by Theorems 4.4 and 4.6.

<u>Theorem 4.14</u>. Let

$$\Sigma = \bigcup_{-1/2<p\le 1/2} \{(p,\zeta) \mid \zeta\in \Sigma_p\} = \bigcup_{-1/2<p\le 1/2} \{(p,\zeta) \mid \pi_p(\zeta)\in \sigma(A_{p,\zeta,r})\} . \tag{4.46}$$

Then $M-\Sigma$ is open in M and

$$(p,\zeta) \to R_{p,\zeta,r} \in B(L_2(\Omega_{0,r})) \tag{4.47}$$

is continuous on $M-\Sigma$.

<u>Theorem 4.15</u>. The mapping

$$(p,\zeta) \to P^{-1}_{p,\zeta,r}\, R_{p,\zeta,r} \in B(L_2(\Omega_{0,r}),L_2^{1,\ell oc}(\Delta,\Omega)) \tag{4.48}$$

is continuous on $M-\Sigma$.

A direct consequence of Theorem 4.15 that is needed below is

<u>Corollary 4.16</u>. Let K be any compact subset of $M-\Sigma$ and let $r' > r > h$. Then there exists a constant $C = C(K,r,r')$ such that

$$\| P^{-1}_{p,\zeta,r}\, R_{p,\zeta,r}\, f\|_{1;\Delta;0,r'} \le C\, \|f\|_{0,r} \tag{4.49}$$

for all $(p,\zeta) \in K$ and all $f \in L_2(\Omega_{0,r})$.

<u>A Limiting Absorption Theorem</u>. In the remainder of this report the point ζ will be restricted to $\overline{M_p^+}$, the closure of M_p^+ in M_p. To simplify the notation points $\zeta \in M_p^+$ will be identified with their images $\pi_p(\zeta) = z \in C - [p^2,\infty)$ and the points of ∂M_p^+ will be denoted by $\lambda \pm i0$, where $\lambda \in [p^2,\infty)$. With this notation the operators

$$P^{-1}_{p,\lambda\pm i\sigma,r}\, R_{p,\lambda\pm i\sigma,r} \in B(L_2(\Omega_{0,r}),L_2^{1,\ell oc}(\Delta,\Omega)) \tag{4.50}$$

are defined and continuous for all $\lambda \pm i\sigma \in \overline{M_p^+} - \Sigma_p$. Note that by Corollary 4.13

$$\sigma(A_p) - \sigma_0(A_p) - T_p \subset \pi_p(\partial M_p^+ - \Sigma_p) \quad (4.51)$$

Now let $f \in L_2(\Omega_{0,r})$ and define

$$u_\pm(\cdot,p,\lambda) = P^{-1}_{p,\lambda\pm i0,r}\, R_{p,\lambda\pm i0,r}\, f \in F_{p,\lambda\pm i0,r} \quad (4.52)$$

Then, in particular,

$$u_\pm(\cdot,p,\lambda) \in D(A_p^{\ell oc}) \text{ , and} \quad (4.53)$$

$$\Delta u_\pm + \lambda u_\pm = f \text{ in } \Omega \quad (4.54)$$

Moreover, $\pi_p(\lambda \pm i0) = \lambda$ for all $\lambda \in \sigma(A_p)$ and

$$\begin{aligned} w_{p+m}(\lambda \pm i0) &= \pm(\lambda - (p+m)^2)^{1/2} \text{ if } \lambda > (p+m)^2 , \\ w_{p+m}(\lambda \pm i0) &= i((p+m)^2 - \lambda)^{1/2} \text{ if } \lambda < (p+m)^2 . \end{aligned} \quad (4.55)$$

Hence, the Fourier series (4.28) of $u_\pm$ have the form

$$\begin{aligned} u_\pm(x,y,p,\lambda) = &\sum_{(p+m)^2<\lambda} c_m^\pm e^{i(p+m)x} e^{\pm iy(\lambda-(p+m)^2)^{1/2}} \\ &+ \sum_{(p+m)^2>\lambda} c_m^\pm e^{i(p+m)x} e^{-y((p+m)^2-\lambda)^{1/2}} \end{aligned} \quad (4.56)$$

Thus u_+ and u_- are the outgoing and incoming solutions, respectively, of the boundary value problem (4.53), (4.54). Moreover, they are uniquely determined by these conditions, by Theorem 2.1, provided

$$\lambda \in \sigma(A_p) - \sigma_0(A_p) - T_p \ . \tag{4.57}$$

The final result of this section is a uniform bound for the functions

$$P^{-1}_{p,\lambda\pm i\sigma,r}\ R_{p,\lambda\pm i\sigma,r}\ f \in L_2^{1,\ell oc}(\Delta,\Omega) \tag{4.58}$$

which may be formulated as follows.

<u>Corollary 4.17</u>. Let $I = [a,b]$ satisfy

$$I \subset \sigma(A_p) - \sigma_0(A_p) - T_p \tag{4.59}$$

and let p, σ_0, r and r' satisfy $-1/2 < p \leq 1/2$, $\sigma_0 > 0$ and $r' > r > h$. Then there exists a constant $C = C(I,p,\sigma_0,r,r')$ such that

$$\| P^{-1}_{p,\lambda\pm i\sigma,r}\ R_{p,\lambda\pm i\sigma,r}\ f \|_{1;\Delta;0,r'} \leq C \| f \|_{0,r} \tag{4.60}$$

for all $\lambda \in I$, $0 \leq \sigma \leq \sigma_0$ and all $f \in L_2(\Omega_{0,r})$.

This result is a direct consequence of Corollary 4.16.

§5. The Eigenfunction Expansions for A_p.

This section presents a construction, based on the limiting absorption theorem of §4, of the diffracted plane wave eigenfunctions $\phi_\pm(X,p+m,q)$ and a derivation of the corresponding eigenfunction expansions for A_p. For brevity the derivation is restricted to the cases for which $\sigma_0(A_p) = \phi$. The modifications that are needed when $\sigma_0(A_p) \neq \phi$ are indicated at the end of the section.

Throughout this section $p \in (-1/2,1/2]$ is fixed, $m \in Z$ and $q > 0$. $\phi_0(X,p+m,q)$ denotes the generalized eigenfunction for $A_{0,p}$; that is, one of the functions (3.25), (3.26). The corresponding outgoing and incoming diffracted plane waves for A_p are characterized by the properties

$$\phi_\pm(\cdot,p+m,q) \in D(A_p^{\ell oc}) \ , \tag{5.1}$$

$$(\Delta + \omega^2(p+m,q))\ \phi_\pm(X,p+m,q) = 0 \text{ in } \Omega \ , \tag{5.2}$$

$$\phi_\pm(X,p+m,q) = \phi_0(X,p+m,q) + \phi_\pm'(X,p+m,q) \ , \ y \geq h \ , \tag{5.3}$$

where ϕ_+' (resp., ϕ_-') is an outgoing (resp., incoming) diffracted plane wave in Ω_h. These properties imply the symmetry relation

$$\phi_-(X,p+m,q) = \overline{\phi_+(X,-p-m,q)} \ . \tag{5.4}$$

Hence it will be sufficient to construct the functions $\phi_+(X,p+m,q)$.

To construct ϕ_+ fix an $r > h$ and introduce a function $j \in C^\infty[0,\infty)$ such that $j'(y) \geq 0$, $0 \leq j(y) \leq 1$, $j(y) \equiv 0$ for $0 \leq y \leq (h + r)/2$ and $j(y) \equiv 1$ for $y \geq r$. Next define the function $\phi_+'(X,p+m,q)$ for all $X \in \Omega$ by

(5.5) $$\phi_+(X,p+m,q) = j(y)\ \phi_0(X,p+m,q) + \phi_+'(X,p+m,q)\ ,\ X \in \Omega\ .$$

Then (5.1), (5.2), (5.3) imply that ϕ_+' is characterized by the properties

(5.6) $$\phi_+'(\cdot,p+m,q) \in D(A_p^{\ell oc})$$

(5.7) $$(\Delta + \omega^2(p+m,q))\ \phi_+'(X,p+m,q) = -M(X,p+m,q) \text{ in } \Omega\ ,$$

(5.8) $\phi_+'(X,p+m,q)$ is an outgoing diffracted plane wave.

The function M in (5.7) is defined for all $X \in R_0^2$, $p + m \in R$ and $q > 0$ by

(5.9)
$$\begin{aligned} M(X,p+m,q) &= (\Delta + \omega^2(p+m,q))\ j(y)\ \phi_0(X,p+m,q) \\ &= j''(y)\ \phi_0(X,p+m,q) + 2\ j'(y)\ D_2\ \phi_0(X,p+m,q) \end{aligned}$$

and has the properties

(5.10) $$M \in C^\infty(R_0^2 \times R \times R_0)\ ,$$

(5.11) $$M(x+2\pi,y,p+m,q) = \exp\{2\pi ip\}\ M(x,y,p+m,q)\ ,$$

(5.12) $$\operatorname{supp} M(\cdot,p+m,q) \subset \{X \mid (h + r)/2 \le y \le r\}\ .$$

It follows that $M(\cdot,p+m,q)|_{\Omega_{0,r}} \in L_2(\Omega_{0,r})$ and hence (5.6), (5.7), (5.8) can be integrated by means of the analytic continuation of the resolvent of A_p defined by (4.50). More generally

(5.13) $$\phi'(\cdot,p+m,q,z) = P_{p,z,r}^{-1}\ R_{p,z,r}\ M(\cdot,p+m,q) \in D(A_p^{\ell oc})$$

and $z \to \phi'(\cdot,p+m,q,z) \in L_2^{1,\ell oc}(\Delta,\Omega)$ is continuous for all $q > 0$ and $z \in \overline{M_p^+} - \Sigma_p$. Hence, $\phi'(\cdot,p+m,p,\lambda+i0) \in D(A_p^{\ell oc})$ satisfies $(\Delta + \lambda)\phi' = 0$ in Ω and the outgoing radiation condition (4.56) for all $\lambda \in [p^2,\infty) - T_p$.

In particular, the solution of (5.6), (5.7), (5.8) is defined by

$$\phi_+'(\cdot,p+m,q) = \phi'(\cdot,p+m,q,\omega^2(p+m,q) + i0) \tag{5.14}$$

for all $q \in R_0 - E_{m,p}$ where

$$E_{m,p} = \{q > 0 \mid \omega^2(p+m,q) \in T_p\} . \tag{5.15}$$

Note that $E_{m,p}$ is a countable subset of $R_0 = (0,\infty)$ with no finite limit points.

The diffracted plane wave $\phi_+(X,p+m,q)$ is defined by (5.5), (5.13) and (5.14) and one has

<u>Theorem 5.1</u>. Let G be a grating domain of the class defined in §1 and let $\sigma_0(A_p) = \phi$. Then there exist unique diffracted plane wave eigenfunctions $\phi_\pm(X,p+m,q)$ for each $p \in (-1/2,1/2]$, $m \in Z$ and $q \in R_0 - E_{m,p}$. Moreover, $q \to \phi_\pm(\cdot,p+m,q) \in L_2^{1,\ell oc}(\Delta,\Omega)$ is continuous for $q \in R_0 - E_{m,q}$.

The uniqueness follows from Theorem 2.1 and $\sigma_0(A_p) = \phi$. The continuity is a consequence of Theorem 4.15.

The functions

$$\phi(X,p+m,q,z) = j(y)\ \phi_0(X,p+m,q) + \phi'(X,p+m,q,z) \in D(A_p^{\ell oc}) , \tag{5.16}$$

which are defined for $p \in (-1/2,1/2]$, $m \in Z$, $q > 0$ and $z \in \overline{M_p^+} - \Sigma_p$ will be used in deriving the eigenfunction expansions for ϕ_+ and ϕ_-. They will be called approximate eigenfunctions of A_p because

$$(\Delta + z)\ \phi(X,p+m,q,z) = (z - \omega^2(p+m,q))\ j(y)\ \phi_0(X,p+m,q) \tag{5.17}$$

and

$$\phi(X,p+m,q,\omega^2(p+m,q) \pm i0) = \phi_\pm(X,p+m,q) \quad . \tag{5.18}$$

<u>Construction of the Spectral Family of A_p</u>. The selfadjoint operator A_p in $L_2(\Omega)$ has a spectral family $\{\Pi_p(\mu) \mid \mu \geq p^2\}$ which is continuous when $\sigma_0(A_p) = \phi$. The spectral measure $\Pi_p(I) = \Pi_p(b) - \Pi_p(a)$ of an interval $I = [a,b]$ will now be calculated by means of Stone's formula

$$\|\Pi_p(I)f\|^2 = \lim_{\sigma\to 0+} \frac{\sigma}{\pi} \int_I \|R(A_p,\lambda \pm i\sigma)\|^2 \, d\lambda \tag{5.19}$$

and the eigenfunctions $\phi_\pm$. Only the main steps of the calculation will be given because a detailed presentation of the analogous calculation for exterior domains was given in [34].

To begin it will be assumed that $I \subset [p^2,\infty) - T_p$ and $f \in L_2^{com}(\Omega)$. Note that if $j(y)$ is the cut-off function of (5.5) then

$$|(1 - j^2(y)) \, R(A_p,z) \, f(X)|^2 \leq \chi_r(y) \, |R(A_p,z) \, f(X)|^2 \tag{5.20}$$

where χ_r is the characteristic function of $[0,r]$. Since $\lim_{\sigma\to 0+} R(A_p,\lambda\pm i\sigma)f$ exists in $L_2(\Omega_{0,r})$, uniformly for $\lambda \in I$, it follows that

$$\int_\Omega (1 - j^2(y)) \, |R(A_p,\lambda\pm i\sigma) \, f(X)|^2 \, dX = O(1) \ , \ \sigma \to 0+ \ , \tag{5.21}$$

uniformly for $\lambda \in I$. Define a linear operator $J : L_2(\Omega) \to L_2(B_0)$ by

$$J \, f(X) = \begin{cases} j(y) \, f(X) \ , & X \in \Omega \\ 0 \ , & X \in B_0 - \Omega \end{cases} \tag{5.22}$$

Then $\|J\| = 1$ and (5.21) implies

$$\|R(A_p,z)f\|^2 = \|J\ R(A_p,z)f\|^2 + O(1)\ ,\ \mathrm{Im}\ z \to 0\ , \tag{5.23}$$

uniformly for Re $z \in I$. Next, Parseval's relation (3.29) for $A_{0,p}$ and (5.23) imply

$$\|R(A_p,z)f\|^2 = \sum_{m\in Z} \|(J\ R(A_p,z)f)_0^{\sim}\ (p+m,\cdot)\|^2 + O(1),\ \mathrm{Im}\ z \to 0, \tag{5.24}$$

uniformly for Re $z \in I$. To relate this to the eigenfunctions $\phi_\pm$ define

$$\tilde{f}(p+m,q,z) = \int_\Omega \overline{\phi(X,p+m,q,\overline{z})}\ f(X)\ dX,\ f \in L_2^{com}(\Omega), \tag{5.25}$$

and note

<u>Lemma 5.2</u>. For all $f \in L_2^{com}(\Omega)$ one has

$$\tilde{f}(p+m,q,z) = (\omega^2(p+m,q) - z)\ (J\ R(A_p,z)f)_0^{\sim}\ (p+m,q)\ . \tag{5.26}$$

A heuristic proof of (5.26) is contained in the following formal calculations, based on (5.17).

$$\begin{aligned} \tilde{f}(p+m,q,z) &= \int_\Omega \overline{R(A_p,\overline{z})(A_p - \overline{z})\ \phi(X,p+m,q,\overline{z})}\ f(X)\ dx \\ &= \int_\Omega \overline{(\omega^2(p+m,q) - z)\ j(y)\ \phi_0(X,p+m,q)}\ R(A_p,z)\ f(X)\ dX \\ &= (\omega^2(p+m,q) - z) \int_{B_0} \overline{\phi_0(X,p+m,q)}\ j(y)\ R(A_p,z)\ f(X)\ dx \\ &= (\omega^2(p+m,q) - z)\ (J\ R(A_p,z)f)_0^{\sim}\ (p+m,q)\ . \end{aligned} \tag{5.27}$$

The calculation is not rigorous because the presence of the term $j\phi_0$ in

(5.16) implies that $\phi(\cdot,p+m,q,z) \notin D(A_p)$. A rigorous but longer proof may be given by the technique of [34, p. 94].

Combining (5.24) and (5.26) gives

$$\|R(A_p,z)f\|^2 = \sum_{m\in Z} \left\| \frac{\tilde{f}(p+m,\cdot,z)}{\omega^2(p+m,\cdot)-z} \right\|^2 + O(1), \text{ Im } z \to 0, \tag{5.28}$$

uniformly for Re $z \in I$. Hence, putting $z = \lambda \pm i\sigma$, multiplying by σ/π and integrating over $\lambda \in I$ gives

$$\begin{aligned} \frac{\sigma}{\pi}\int_I \|R(A_p,\lambda\pm i\sigma)f\|^2\, d\lambda &= \frac{\sigma}{\pi}\int_I \sum_{m\in Z}\int_0^\infty \frac{|\tilde{f}(p+m,q,\lambda\pm i\sigma)|^2}{(\lambda-\omega^2(p+m,q))^2+\sigma^2}\, dq\, d\lambda + O(\sigma) \\ &= \sum_{m\in Z}\int_0^\infty \left(\frac{\sigma}{\pi}\int_I \frac{|\tilde{f}(p+m,q,\lambda\pm i\sigma)|^2}{(\lambda-\omega^2(p+m,q))^2+\sigma^2}\, d\lambda\right) dq + O(\sigma) \end{aligned} \tag{5.29}$$

by Fubini's theorem. The determination of $\Pi_p(I)$ will be completed by calculating the limit for $\sigma \to 0$ of the last equation. Note that the continuity of the approximate eigenfunctions (5.16) for $q > 0$, $z \in \overline{M_p^+} - \Sigma_p$ (cf. (5.13)) implies that $\tilde{f}(p+m,q,\lambda\pm i\sigma)$ is continuous for $q > 0$, $\lambda \in [p^2,\infty) - T_p$, $\sigma \geq 0$. Thus if one defines

$$\tilde{f}_\pm(p+m,q) = \tilde{f}(p+m,q,\omega^2(p+m,q) \mp i0), \quad q \in R_0 - E_{m,p} \tag{5.30}$$

then for all $f \in L_2^{com}(\Omega)$

$$\tilde{f}_\pm(p+m,q) = \int_\Omega \overline{\phi_\pm(X,p+m,q)}\, f(X)\, dx \tag{5.31}$$

and

$$\tilde{f}_\pm(p+m,\cdot) \in C(R_0 - E_{m,p}) . \tag{5.32}$$

The calculation of the limiting form of (5.29) will be based on the following two lemmas.

<u>Lemma 5.3</u>. For every $f \in L_2^{com}(\Omega)$ and every closed interval $I \subset [p^2,\infty) - \mathcal{T}_p$ one has

$$(5.33) \qquad \lim_{\sigma\to 0+} \frac{\sigma}{\pi} \int_I \frac{|\tilde{f}(p+m,q,\lambda\pm i\sigma)|^2}{(\lambda-\omega^2(p+m,q))^2+\sigma^2}\, d\lambda = \chi_I(\omega^2(p+m,q))\,|\tilde{f}_\mp(p+m,q)|^2$$

for all $q \in R_0^2 - \mathcal{E}_{m,p}$ where $\chi_I(\lambda)$ is the characteristic function of I, normalized so that $\chi_I(a) = \chi_I(b) = 1/2$.

Lemma 5.3 follows from the continuity of $\tilde{f}(p+m,q,\lambda\pm i\sigma)$ and well-known properties of the Poisson kernels; cf. [34, p. 101].

<u>Lemma 5.4</u>. For every $f \in L_2^{com}(\Omega)$, every closed interval $I \subset [p^2,\infty) - \mathcal{T}_p$ and every $\sigma_0 > 0$ there exists a constant $C = C(f,I,\sigma_0)$ such that

$$(5.34) \qquad \sum_{m\in Z} \int_0^\infty |\tilde{f}(p+m,q,\lambda\pm i\sigma)|^2\, dq \le C$$

for all $p \in (-1/2,1/2]$, $\lambda \in I$ and $\sigma \in [0,\sigma_0]$.

This result is the analogue of [34, Lemma 6.8, p. 103]. A full proof, based on Corollary 4.17, is given in [38].

The limit of equation (5.29) for $\sigma \to 0$ may now be calculated. Lemma 5.3 gives the limits of the inner integrals in (5.29). Term-wise passage to the limit can be justified by Lemma 5.4 and Lebesgue's dominated convergence theorem; see [34] for details. The result is, by (5.19),

$$(5.35) \qquad \|\Pi_p(I)f\|^2 = \sum_{m\in Z} \int_0^\infty \chi_I(\omega^2(p+m,q))\ |\tilde{f}_\pm(p+m,q)|^2\, dq$$

for all $f \in L_2^{com}(\Omega)$ and $I \subset [p^2,\infty) - T_p$ where $\tilde{f}_\pm(p+m,q)$ is given by (5.31).

The Eigenfunction Expansions for A_p. The eigenfunction expansions for A_p based on $\phi_+(X,p+m,q)$ and $\phi_-(X,p+m,q)$ can be derived from (5.35) and the spectral theorem by standard methods; cf. [34, p. 109ff]. Only the results are given here. Details may be found in [34] and [38].

To begin note that since $\sigma_0(A_p) = \phi$ the restriction $I \subset [p^2,\infty) - T_p$ can be dropped; (5.35) is valid for $f \in L_2^{com}(\Omega)$ and all $I \subset [p^2,\infty)$. Making $I \to [p^2,\infty)$ then gives the Parseval relation

$$\|f\|^2_{L_2(\Omega)} = \sum_{m\in Z} \|\tilde{f}_\pm(p+m,\cdot)\|^2_{L_2(R_0)} \tag{5.36}$$

for all $f \in L_2^{com}(\Omega)$. Together with (5.32) this implies that for $f \in L_2^{com}(\Omega)$,

$$\tilde{f}_\pm(p+m,\cdot) \in C(R_0 - E_{m,p}) \cap L_2(R_0). \tag{5.37}$$

A standard density argument then implies

Theorem 5.5. For all $f \in L_2(\Omega)$ the limits

$$\tilde{f}_\pm(p+m,q) = L_2(R_0)\text{-}\lim_{M\to\infty} \int_{\Omega_{0,M}} \overline{\phi_\pm(X,p+m,q)}\, f(X)\, dX \tag{5.38}$$

exist and (5.35), (5.36) are valid for all $f \in L_2(\Omega)$.

An eigenfunction representation of the spectral family can now be obtained from (5.35) by the usual polarization and factorization arguments. In this way one obtains

Theorem 5.6. For all $f \in L_2(\Omega)$ one has

$$\Pi_p(\mu)\, f(X) = \sum_{(p+m)^2\le\mu} \int_0^{(\mu-(p+m)^2)^{1/2}} \phi_\pm(X,p+m,q)\, \tilde{f}_\pm(p+m,q)\, dq \tag{5.39}$$

and hence

$$(5.40) \qquad f(X) = L_2(\Omega)\text{-}\lim_{M\to\infty} \sum_{|m|\le M} \int_0^M \phi_\pm(X,p+m,q)\, \tilde{f}_\pm(p+m,q)\, dq \ .$$

Finally, define linear operators

$$(5.41) \qquad \Phi_{\pm,p} : L_2(\Omega) \to \sum_{m\in Z} \oplus\, L_2(R_0)$$

by

$$(5.42) \qquad \Phi_{\pm,p}\, f = \{\tilde{f}_\pm(p+m,\cdot) \mid m \in Z\}$$

Then $\Phi_{+,p}$ and $\Phi_{-,p}$ are spectral mappings for A_p in the sense of

Theorem 5.7. For every bounded, Lebesgue-measurable function $\Psi(\lambda)$ defined on $p^2 \le \lambda < \infty$ one has

$$(5.43) \qquad (\Phi_{\pm,p}\, \Psi(A_p) f)_m = \Psi(\omega^2(p+m,\cdot))(\Phi_{\pm,p} f)_m \ , \ m \in Z$$

where $\Psi(A_p)$ is defined by the spectral theorem.

Finally, the orthogonality and completeness of the generalized eigenfunctions $\phi_\pm$ is expressed by

Theorem 5.8. The operators $\Phi_{+,p}$ and $\Phi_{-,p}$ are unitary.

It is clear from Parseval's relation (5.36) that $\Phi_{\pm,p}$ are isometries which proves the completeness relation

$$(5.44) \qquad \Phi^*_{\pm,p}\, \Phi_{\pm,p} = 1 \ .$$

The surjectivity of $\Phi_{\pm,p}$ which is equivalent to the orthogonality relation

$$(5.45) \qquad \Phi_{\pm,p}\, \Phi^*_{\pm,p} = 1$$

is not a consequence of the spectral theorem. A proof of (5.45) by the method introduced in [34, p. 112ff] is given in [38].

Operators A_p that have Point Spectrum. It was shown in §4 that, in general, $\sigma_0(A_p)$ is discrete. Let $\mathcal{H}_0$ be the subspace of $L_2(\Omega)$ spanned by the eigenvectors of A_p and let $\dim \mathcal{H}_0 = N(p) - 1 \leq \infty$. Let $\{\lambda_j(p) \mid 1 \leq j < N(p)\}$ be the eigenvalues, repeated according to their multiplicity and enumerated so that $\lambda_j(p) \leq \lambda_{j+1}(p)$. Let $\{\phi_j(X,p) \mid 1 \leq j < N(p)\}$ be a corresponding orthonormal set of eigenfunctions.

Proceeding as before it is found that the diffracted plane waves $\phi_\pm(X,p+m,q)$ can be constructed and Theorem 5.1 holds with

$$E_{m,p} = \{q > 0 \mid \omega^2(p+m,q) \in T_p \cup \sigma_0(A_p)\} \tag{5.46}$$

which is still a countable set with no finite limit points. Similarly, the spectral family $\{\Pi_p(\mu)\}$ still satisfies (5.35) for $f \in L_2^{com}(\Omega)$ if $I \subset [p^2,\infty) - T_p - \sigma_0(A_p)$. It follows that $\Pi_p(\mu)$ differs from (5.39) only by the projection

$$\sum_{\lambda_j(p)\leq\mu} \phi_j(X,p)\, \tilde{f}_j(p) \ , \ \tilde{f}_j(p) = (\phi_j(\cdot,p),f)_{L_2(\Omega)} \ . \tag{5.47}$$

and Parseval's relation and the eigenfunction expansion become

$$\|f\|^2 = \sum_{j=1}^{N-1} |\tilde{f}_j(p)|^2 + \sum_{m\in Z} \|\tilde{f}_\pm(p+m,\cdot)\|^2 \ , \ f \in L_2(\Omega) \ . \tag{5.48}$$

and

$$f(X) = \sum_{j=1}^{N-1} \phi_j(X,p)\, \tilde{f}_j(p) + \sum_{m\in Z} \int_0^\infty \phi_\pm(X,p+m,q)\, \tilde{f}_\pm(p+m,q)\, dq \ , \tag{5.49}$$

convergent in $L_2(\Omega)$. The form of the spectral family implies that A_p has no singular continuous spectrum : $L_2(\Omega) = \mathcal{H}_0 \oplus \mathcal{H}_{ac}$, where $\mathcal{H}_{ac}$ is the subspace of absolute continuity for A_p [17, Ch. X]. Finally, Theorem 5.8 must be modified to state that $\Phi_{+,p}$ and $\Phi_{-,p}$ are partial isometries with initial set $\mathcal{H}_{ac}$ and final set $\Sigma \oplus L_2(R_0)$:

(5.50)
$$\Phi^*_{\pm,p}\, \Phi_{\pm,p} = P_{ac} \;, \quad \Phi_{\pm,p}\, \Phi^*_{\pm,p} = 1$$

where P_{ac} is the orthogonal projection of $L_2(\Omega)$ onto $\mathcal{H}_{ac}$.

§6. The Rayleigh-Bloch Wave Expansions for A.

This section presents a construction, based on the results of §5, of the R-B diffracted plane wave eigenfunctions $\psi_\pm(X,p,q)$ and a derivation of the corresponding R-B wave expansions for A. For brevity the derivation is restricted to the cases for which A has no surface waves; that is, $\sigma_0(A_p) = \phi$ for all p. The modifications that are needed when there are surface waves are indicated at the end of the section.

In this section $\psi_0(X,p,q)$ denotes the R-B wave eigenfunction for A_0; that is, one of the functions (1.33), (1.34). The defining properties of $\psi_\pm(X,p,q)$ can then be written

(6.1) $$\psi_\pm(\cdot,p,q) \in D(A^{\ell oc}) \ , \ (p,q) \in R_0^2 \ ,$$

(6.2) $$(\Delta + \omega^2(p,q))\ \psi_\pm(X,p,q) = 0 \text{ in } G \ ,$$

(6.3) $$\psi_\pm(X,p,q) = \psi_0(X,p,q) + \psi_\pm'(X,p,q) \text{ in } R_h^2 \ ,$$

where ψ_+' (resp., ψ_-') is an outgoing (resp., incoming) R-B wave for G.

The construction of $\psi_\pm$ will be based on the discussion at the end of §3. Thus if $(p,q) \in R_0^2$ and $p = p_0 + m$ where $p_0 \in (-1/2,1/2]$ and $m \in Z$ then $\psi_\pm(X,p,q)$ are defined by

(6.4) $$\psi_\pm(X,p,q) = \mathcal{O}^{p_0}\phi_\pm(X,p_0+m,q) \ ,$$

or, more explicitly,

(6.5) $$\psi_\pm(x,y,p,q) = \exp\{2\pi i\ell p_0\}\ \phi_\pm(x-2\pi\ell,y,p_0+m,q) \ , \ (x,y) \in \Omega^{(\ell)} \ .$$

Theorem 5.1 then implies

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<u>Theorem 6.1</u>. Let G be a grating domain of the class defined in §1 and let $A = A(G)$ have no surface waves. Then there exist unique R-B diffracted plane waves $\psi_{\pm}(X,p,q)$ for each $(p,q) \in R_0^2 - E$, where E is the exceptional set (2.30). Moreover, the mapping $(p,q) \to \psi_{\pm}(\cdot,p,q) \in L_2^{1,\ell oc}(\Delta,G)$ is continuous for $(p,q) \in R_0^2 - E$.

The principal step in the proof of Theorem 6.1 is to show that $\psi_{\pm}$, defined piece-wise by (6.5), satisfies (6.1). This may be done by a simple distribution-theoretic calculation based on the p-periodic boundary condition for $\phi_{\pm}$. Details are given in [38]. The uniqueness statement follows from Theorem 2.1 since $\sigma_0(A_p) = \phi$ for all p is assumed.

The R-B wave expansions for A will now be derived from the eigenfunction expansions for A_p of §5. The first step is to establish Parseval's relation for A. The special case of functions $f \in L_2^{com}(G)$ is treated first.

<u>Theorem 6.2</u>. For all $f \in L_2^{com}(G)$ define

$$(6.6) \qquad \hat{f}_{\pm}(p,q) = \int_G \overline{\psi_{\pm}(X,p,q)}\, f(X)\, dX \ , \ (p,q) \in R_0^2 - E \ .$$

Then

$$(6.7) \qquad \hat{f}_{\pm} \in C(R_0^2 - E) \cap L_2(R_0^2) \ , \text{ and}$$

$$(6.8) \qquad \|f\|_{L_2(G)} = \|\hat{f}_{\pm}\|_{L_2(R_0^2)} \ .$$

<u>Proof</u>. The finiteness of $\hat{f}_{\pm}(p,q)$ for $(p,q) \in R_0^2 - E$ and the property $\hat{f}_{\pm} \in C(R_0^2 - E)$ follow from the last statement of Theorem 6.1. To establish the rest of the theorem note the following identity for functions $f \in L_2^{com}(G)$ and points $(p,q) \in R_0^2 - E$.

$$
\begin{aligned}
\hat{f}_{\pm}(p,q) &= \int_G \overline{\psi_{\pm}(X,p,q)}\, f(X)\, dX \\
&= \sum_{\ell\in Z} \int_{\Omega(\ell)} \overline{\psi_{\pm}(X,p,q)}\, f(X)\, dX \\
&= \sum_{\ell\in Z} \int_{\Omega} \overline{\psi_{\pm}(x+2\pi\ell,y,p,q)}\, f(x+2\pi\ell,y)\, dxdy \\
&= \sum_{\ell\in Z} \int_{\Omega} \overline{\phi_{\pm}(x,y,p,q)}\, e^{-2\pi i\ell p}\, f(x+2\pi\ell,y)\, dxdy \\
&= \int_{\Omega} \overline{\phi_{\pm}(x,y,p,q)} \left(\sum_{\ell\in Z} e^{-2\pi i\ell p}\, f(x+2\pi\ell,y)\right) dxdy \\
&= \int_{\Omega} \overline{\phi_{\pm}(x,y,p,q)}\, F(x,y,p)\, dxdy
\end{aligned} \tag{6.9}
$$

where

$$
F(x,y,p) = \sum_{\ell\in Z} e^{-2\pi i\ell p}\, f(x+2\pi\ell,y)\ , \quad (x,y) \in \Omega\ . \tag{6.10}
$$

Note that all the sums in (6.9) are finite when $f \in L_2^{com}(G)$. Moreover, (6.10) is a Fourier series in p with a fixed finite number of non-zero terms for all $(x,y) \in \Omega$.

Equation (6.9) establishes a relation between the eigenfunction expansions for A and A_p. Thus replacing p in (6.9) by p + m with $p \in (-1/2,1/2]$ and $m \in Z$ one has

$$
\hat{f}_{\pm}(p+m,q) = \tilde{F}_{\pm}(p+m,q,p) \tag{6.11}
$$

in the notation of §5. In particular, Parseval's relation for A_p, applied to $F(\cdot,p)$, and (6.11) gives

$$(6.12) \qquad \int_{\Omega} |F(X,p)|^2 \, dX = \sum_{m\in Z} \int_0^{\infty} |\hat{f}_{\pm}(p+m,q)|^2 \, dq$$

Noting the continuity of $p \to F(\cdot,p) \in L_2(\Omega)$ and integrating (6.12) over $p \in (-1/2,1/2]$ gives

$$(6.13) \qquad \begin{aligned} \int_{-1/2}^{1/2} \int_{\Omega} |F(X,p)|^2 \, dX \, dp &= \sum_{m\in Z} \int_{-1/2}^{1/2} \int_0^{\infty} |\hat{f}_{\pm}(p+m,q)|^2 \, dqdp \\ &= \int_{R_0^2} |\hat{f}_{\pm}(p,q)|^2 \, dpdq = \|\hat{f}_{\pm}\|^2_{L_2(R_0^2)} \ . \end{aligned}$$

In particular, $\hat{f}_{\pm} \in L_2(R_0^2)$ which completes the proof of (6.7). To verify (6.8) note that Parseval's formula for Fourier series implies that

$$(6.14) \qquad \int_{-1/2}^{1/2} |F(X,p)|^2 \, dp = \sum_{\ell\in Z} |f(x+2\pi\ell,y)|^2 \ , \ X \in \Omega \ ,$$

where the sum has a fixed finite number of terms for all $X \in \Omega$. Integrating (6.14) over $X \in \Omega$ and applying Fubini's theorem gives

$$(6.15) \qquad \begin{aligned} \int_{-1/2}^{1/2} \int_{\Omega} |F(X,p)|^2 \, dX \, dp &= \sum_{\ell\in Z} \int_{\Omega} |f(x+2\pi\ell,y)|^2 \, dX \ . \\ &= \sum_{\ell\in Z} \int_{\Omega(\ell)} |f(X)|^2 \, dX \\ &= \int_G |f(X)|^2 \, dX = \|f\|^2_{L_2(G)} \end{aligned}$$

Combining (6.13) and (6.15) gives (6.8).

The extension of Parseval's relation to all $f \in L_2(G)$ follows from Theorem 6.2 by a standard technique using the denseness of $L_2^{com}(G)$ in $L_2(G)$. Thus, writing

$$G_M = G \cap \{X \mid x^2 + y^2 < M^2\} , \tag{6.16}$$

one has

Corollary 6.3. The limits

$$\hat{f}_\pm(p,q) = L_2(R_0^2)\text{-}\lim_{M\to\infty} \int_{G_M} \overline{\psi_\pm(X,p,q)}\, f(X)\, dX \tag{6.17}$$

exist and Parseval's relation (6.8) holds for all $f \in L_2(G)$.

A representation of the spectral family $\{\Pi(\mu) \mid \mu \geq 0\}$ of the grating propagator A will now be derived from Corollary 6.3. The key fact is described by

Theorem 6.4. The resolvent $R(A,z) = (A - z)^{-1}$ of the grating propagator A satisfies the relation

$$\|R(A,z)f\|^2_{L_2(G)} = \int_{R_0^2} \frac{|\hat{f}_\pm(p,q)|^2}{|\omega^2(p,q)-z|^2}\, dpdq \tag{6.18}$$

for all $f \in L_2(G)$ and all $z \in C - [0,\infty)$.

To prove Theorem 6.4 it is enough to verify (6.18) for all $f \in L_2^{com}(G)$. The idea for doing this is to define

$$u(X) = R(A,z)\, f(X) \tag{6.19}$$

and to apply Parseval's relation to $v_M = \phi_M u$ where $\phi_M \in C_0^\infty(R^2)$. For a suitable choice of ϕ_M one has

$$v_M = R(A,z)(f + g_M) \tag{6.20}$$

where

$$g_M = -2\nabla u \cdot \nabla\phi_M - u\,\Delta\phi_M \tag{6.21}$$

and

$$\hat{v}_{M\pm}(p,q) = (\hat{f}_\pm(p,q) + \hat{g}_{M\pm}(p,q))/\omega^2(p,q) - z \tag{6.22}$$

whence

$$\|\phi_M R(A,z)f\| = \|(\hat{f}_\pm + \hat{g}_{M\pm})/\omega^2 - z\| . \tag{6.23}$$

Passage to the limit $M \to \infty$ then gives (6.18). For the case of the Dirichlet boundary condition one may take $\phi_M(X) = \psi(|X| - M)$ where $\psi \in C^\infty(R)$ satisfies $\psi(\tau) \equiv 1$ for $\tau \le 0$ and $\psi(\tau) \equiv 0$ for $\tau \ge 1$. For the case of the Neumann boundary condition ϕ_M must be chosen more carefully, using the condition $G \in S$, to ensure that v_M satisfy the boundary condition. The details of the construction are given in [38].

The R-B wave expansions for A follow easily from Corollary 6.3 and Theorem 6.4. They are formulated as

Theorem 6.5. For all $f \in L_2(G)$ the spectral family $\{\Pi(\mu) \mid \mu \ge 0\}$ of A satisfies

$$\Pi(\mu)\ f(X) = \int_{D_\mu} \psi_\pm(X,p,q)\ \hat{f}_\pm(p,q)\ dpdq \tag{6.24}$$

where

$$D_\mu = R_0^2 \cap \{(p,q) \mid p^2 + q^2 \le \mu\} \tag{6.25}$$

In particular, every $f \in L_2(G)$ has the R-B wave expansion

(6.26) $$f(X) = L_2(G)\text{-}\lim_{M\to\infty} \int_{D_M} \psi_{\pm}(X,p,q)\, \hat{f}_{\pm}(p,q)\, dpdq \; .$$

The relation (6.24) is a direct consequence of the relation

(6.27) $$\| \Pi(I) f \|^2_{L_2(G)} = \int_{R^2} \chi_I(\omega^2(p,q))\, |\hat{f}_{\pm}(p,q)|^2\, dpdq$$

where I is a subinterval of $[0,\infty)$ with characteristic function χ_I. (6.27) follows easily from (6.18) and Stone's formula. Note that (6.27) implies the absolute continuity of the grating propagators.

To formulate the orthogonality and completeness relations for the R-B wave expansions define linear operators

(6.28) $$\Phi_{\pm} : L_2(G) \to L_2(R_0^2)$$

by

(6.29) $$\Phi_{\pm}\, f = \hat{f}_{\pm} \; .$$

Then Φ_+ and Φ_- are spectral mappings for A in the sense of

Theorem 6.6. For every bounded, Lebesgue-measurable function $\Psi(\lambda)$ defined on $0 \leq \lambda < \infty$

(6.30) $$\Phi_{\pm}\, \Psi(A) = \Psi(\omega^2(\cdot))\, \Phi_{\pm}$$

where $\Psi(A)$ is defined by the spectral theorem.

Moreover, one has

Theorem 6.7. The R-B wave expansions are orthogonal and complete in the sense that Φ_+ and Φ_- are unitary operators:

$$\Phi_{\pm}^{*}\,\Phi_{\pm} = 1 \text{ and } \Phi_{\pm}\,\Phi_{\pm}^{*} = 1 \ . \tag{6.31}$$

Relations (6.30) and the completeness relation $\Phi_{\pm}^{*}\,\Phi_{\pm} = 1$ follow easily from the spectral theorem. The orthogonality relation $\Phi_{\pm}\,\Phi_{\pm}^{*} = 1$ can be deduced from the corresponding property of $\Phi_{\pm p}$, Theorem 5.8. Indeed, it is sufficient to prove that

$$(\Phi_{\pm}\,\Phi_{\pm}^{*}f - f, f) = 0 \tag{6.32}$$

for all f in a dense subset of $L_2(R_0^2)$. This may be verified by direct calculation using $f \in C_0^{\infty}(R_0^2 - E)$ and the orthogonality relation for $\Phi_{\pm p}$. The details are given in [38].

Operators A that admit R-B Surface Waves. It was shown in §2 that for each $p \in (-1/2, 1/2]$ A may have R-B surface waves $\psi_j(X,p)$ and eigenvalues $\lambda_j(p)$ with x-momentum p. The functions $\phi_j(X,p) = \psi_j(X,p)|_{\Omega}$ are precisely the eigenfunctions of A_p. The principal difficulty in constructing an eigenfunction expansion for A in this case is in constructing families of R-B surface waves $\psi_j(X,p)$ and eigenvalues $\lambda_j(p)$ whose dependence on p is sufficiently regular. The "axiom of choice" definition (independent choice for each p) in inadequate to give even measurability in p. This was pointed out in the author's paper on the analogous, but simpler, case of Bloch waves in crystals [36].

If ∂G is a union of smooth curves (class C^3) then the Green's functions (4.44), (4.45) can be used to construct an integral equation for the eigenfunctions $\phi_j(X,p)$. In this case the method of [36] can be used to construct "almost holomorphic" families $\{\phi_j(X,p)\}$.

In the general case there is a one-to-one correspondence between eigenfunctions $\phi_j(X,p)$ of A_p and eigenfunctions $\theta_j(X,p)$ of $A_{p,\zeta,r}$ with eigenvalues $\pi_p(\zeta) \in [p^2,\infty)$ given by $\theta_j(\cdot,p) = P_{p,\zeta,r}\, \phi_j(\cdot,p)$. The eigenvalues of $A_{p,\zeta,r}$ are isolated, with finite multiplicity, and may be studied by the methods of analytic perturbation theory (Kato [17, Ch. 7]). These problems will not be pursued here.

If a sufficiently regular family of R-B surface waves for A has been constructed the eigenfunction expansions for A may be derived by the method introduced above. Thus, defining $\psi_j(X,p) \equiv 0$ when $j \geq N(p)$, equation (6.12) must be replaced by

$$\int_\Omega |F(X,p)|^2\, dX = \sum_{j=1}^{\infty} |\hat{f}_j(p)|^2 + \sum_{m\in Z} \int_0^\infty |\hat{f}_\pm(p+m,q)|^2\, dq \tag{6.33}$$

where

$$\hat{f}_j(p) = \int_G \overline{\psi_j(X,p)}\, f(X)\, dX \ . \tag{6.34}$$

Integration over $p \in (-1/2,1/2]$ gives the Parseval relation

$$\|f\|^2_{L_2(G)} = \sum_{j=1}^{\infty} \|\hat{f}_j\|^2_{L_2(-1/2,1/2)} + \|\hat{f}_\pm\|^2_{L_2(R_0^2)} \ . \tag{6.35}$$

The corresponding representation of the spectral family is

$$\begin{aligned} \Pi(\mu)\, f(X) &= \int_{-1/2}^{1/2} \sum_{\lambda_j(p)\leq\mu} \psi_j(X,p)\, \hat{f}_j(p)\, dp \\ &\quad + \int_{D_\mu} \psi_\pm(X,p,q)\, \hat{f}_\pm(p,q)\, dpdq \ . \end{aligned} \tag{6.36}$$

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§7. Concluding Remarks.

It is clear that the methods developed in this report are applicable to diffraction gratings in R^3 (and in R^n, $n > 3$). They are also applicable to gratings with holes, as in Alber [3] where the grating $R^n - G$ is a periodic structure contained in a slab $R^n_{0,h}$ and G is connected. The changes needed to treat these cases are primarily notational. The same methods can also be applied to the physically important cases of dielectric gratings in electromagnetic theory and elastic gratings in acoustics.

The most important unsolved problems for diffraction gratings concern the R-B surface waves. Gratings that admit such surface waves would presumably be good waveguides for signals generated near the grating surface. Geometric criteria for the existence and non-existence of such waves would be of great interest for applications.

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13. ABSTRACT

Abstract.

Plane diffraction gratings with period 2π lying in a strip $0 < y < h$ in the x,y-plane are studied. A Rayleigh-Bloch (R-B) wave for a grating is the response $\psi_+(x,y,p,q)$ to a plane wave $(2\pi)^{-1}\exp\{i(px - qy)\}$ incident from $y > h$ ($p \in \mathbb{R}$, $q > 0$). Thus $(\Delta + (p^2 + q^2))\,\psi_+ = 0$ in the domain G above the grating, ψ_+ satisfies the Dirichlet or Neumann boundary condition on ∂G and for $y > h$

$$\psi_+(x,y,p,q) = (2\pi)^{-1} \exp\{i(px - qy)\}$$

$$+ \sum_{(p+\ell)^2 < p^2+q^2} c_\ell^{+}(p,q) \exp\{i(p_\ell x + q_\ell y)\}$$

$$+ \sum_{(p+\ell)^2 \geq p^2+q^2} c_\ell^{+}(p,q) \exp\{i\, p_\ell x - ((p+\ell)^2 - p^2 - q^2)^{1/2}\, y\}$$

where $(p_\ell, q_\ell) = (p + \ell, (p^2 + q^2 - (p + \ell)^2)^{1/2})$ and the summations are over all integers ℓ satisfying the indicated inequalities. The paper presents a construction of R-B waves and a proof that $\{\psi_+(x,y,p,q) \mid p \in \mathbb{R},\ q > 0\}$ is a complete orthogonal family in $L_2(G)$ in the sense of the Plancherel theory.

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